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The X-ray Diffraction Spikes of Diamond

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The theory of the anomalous X-ray reflexions from certain diamonds is worked out on the assumption that they are produced by the random occurrence of an abnormal spacing in the [100] direction, as suggested by Frank. The calculation is in fair agreement with observed results. The defects are found, however, not to be associated with the occurrence of silicon as an impurity in diamond, nor has any other plausible explanation of their occurrence been found.

1. Introduction

The anomalous X-ray reflexions from certain diamonds have been studied a number of times since their discovery by Raman & Nilakantan (1940), the most recently published experimental work being that of Hoerni & Wooster (1955). Hoerni & Wooster found that the anomalous reflexions have the form of spikes in reciprocal space and that 'in any given reciprocal plane parallel to a face (100) the spikes perpendicular to that plane which pass through the various points lying in the plane have the same spike magnitude'. These relative 'spike magnitudes' were found to be as follows:

Index h	0	1	2	3	4	5
Relative magnitude	0	100	75	5	30	0 ?

The 010 and 001 spike intensities are similarly correlated with the indices k and l respectively. The intensity along a spike was found to decrease as $R^{-2\cdot2}$ with distance R from the reciprocal-lattice point.

Attempts to explain the spikes have postulated the occurrence of laminar defects with equal frequency on the planes (100), (010) and (001). Hoerni & Wooster assumed that planes of carbon atoms occurred with an abnormal electron distribution. It has been shown by Frank (1956) that a segregation of impurity atoms (probably silicon) on (100) planes is sufficient qualitatively to explain the observations. Frank's calculations for a one-dimensional crystal containing impurity atoms show that the occasional occurrence of a unit-cell dimension of about four-thirds the normal value produces roughly the observed spike magnitudes, except that the calculated intensity is too high for $h \geq 4$. It was suggested that a calculation which took into account a slight non-uniformity of spacing across the area of a segregated sheet would give better agreement. Frank's calculations are based on a very simplified model, and do not give a relation between the absolute intensity of the spikes and the concentration of impurity atoms required to produce them.

We have made a more rigorous calculation of the consequences for diffraction of a defect of this kind, and have obtained a relation between the spike intensity and the probability of occurrence of a defect. We have also measured the spike intensity experimentally, and it appears to be too great to be accounted for by a segregation of impurity atoms. Nevertheless, the occurrence of a defect of the kind suggested by Frank (from whatever cause) gives quite fair agreement with the observed spike magnitudes and accounts well for the variation of the intensity of the (111) spike with distance from the reciprocal-lattice point.

2. Theory

We will take the defect to consist of the random occurrence (in the [001] direction), with probability α, of a unit cell separated from its neighbour on one side by a gap of length δ. No assumption is made as to the cause of this abnormal spacing, and the possible change in scattering factor of atoms in an abnormal unit cell is not taken into account. (Frank's calculation shows that near a reciprocal-lattice point the intensity depends predominantly on the displacement of all subsequent planes by the defect, and not on a change in scattering factor at the defect.) Clearly a displacement δ can occur with equal probability between any of four non-equivalent layers of atoms in the diamond structure. To simplify the algebra we take the displacement as always occurring at the same place in the unit cell, that is, if we label the layers 0, 1, 2 and 3 the displacement occurs only between layers 3 and 0 say. It is shown in an Appendix that the removal of this restriction does not materially affect results obtained in this section.

The following treatment is simply a generalization and adaptation of that of Large (1957), who considered the problem of the power spectrum of a random sequence of pulses. We do not at first restrict ourselves to the kind of defect mentioned above, but assume simply that the average distance between equivalent points of successive unit cells in the z direction is $\bar{a}$ and that there is a distribution about the average governed by some probability function. All unit cells are taken to have the same structure factor F. The crystal is taken to be a rectangular parallelopiped of dimensions N_1a, N_2a and N_3a. Let ξ, η, ζ be reciprocal-space coordinates such that $h = 1$ corresponds to $\zeta = 1/a$. The Fourier transform of the crystal is then given by

$$G(\xi, \eta, \zeta) = F\frac{\sin N_1\pi\xi a}{\sin \pi\xi a}\frac{\sin N_2\pi\eta a}{\sin \pi\eta a}\left(\sum_0^{N_3-1} \exp\,(2\pi i\zeta d_n)\right), \quad (1)$$

where d_n is the distance from the crystal origin to the origin of the nth unit cell along the z axis.

Therefore we have

$$\begin{aligned}|G|^2 = F^2\left(\frac{\sin N_1\pi\xi a}{\sin \pi\xi a}\frac{\sin N_2\pi\eta a}{\sin \pi\eta a}\right)^2 & \\ \{N_3+(N_3-1)\exp\,[2\pi i\zeta\bar{a}]\,\overline{\exp\,[2\pi i\zeta\varepsilon_n]} & \\ +(N_3-2)\exp\,[4\pi i\zeta\bar{a}]\,\overline{\exp\,[2\pi i\zeta(\varepsilon_n+\varepsilon_{n+1})]} & \\ +\text{etc.}+\text{complex conjugate}\}\,, & \quad (2)\end{aligned}$$

where we have written $d_{n+1}-d_n = \bar{a}+\varepsilon_n$, and the bar denotes an average over all values of n. Except for a perfect crystal, for which $\varepsilon_n = 0$, we can approximate by putting all factors (N_3-1), (N_3-2) etc. equal to N_3. We also note that

$$\overline{\exp\,[2\pi i\zeta\varepsilon_n]} = \int_{-\infty}^{+\infty} p(\varepsilon)\exp\,[2\pi i\zeta\varepsilon]\,d\varepsilon\,, \quad (3)$$

where $p(\varepsilon)$ is the probability distribution function governing the variation in spacing. Equation (3) is thus the Fourier transform of $p(\varepsilon)$, for which we write $q(\zeta)$. Furthermore

$$\overline{\exp\,[2\pi i\zeta(\varepsilon_n+\varepsilon_{n+1}+\ldots+\varepsilon_{n+m})]} = q(\zeta)^{m+1}\,. \quad (4)$$

Writing K^2 as an abbreviation for

$$\left(\frac{\sin N_1\pi\xi a}{\sin \pi\xi a}\frac{\sin N_2\pi\eta a}{\sin \pi\eta a}\right)^2,$$

and $Q(\zeta) = q(\zeta)\exp\,[2\pi i\zeta\bar{a}]$, we thus have

$$\begin{aligned}|G|^2 &= K^2F^2N_3\{1+Q(\zeta)+Q(\zeta)^2+\ldots \\ &\qquad +Q^*(\zeta)+Q^*(\zeta)^2+\ldots\} \\ &= K^2F^2N_3\left(\frac{1-QQ^*}{1+QQ^*-Q-Q^*}\right)\,. \quad (5)\end{aligned}$$

Returning now to the particular situation where there is a probability α of a spacing $a+\delta$, and $(1-\alpha)$ of a spacing a, we have

$$\bar{a} = a+\alpha\delta$$

and $p(\varepsilon)$ consists of a peak of weight α at $a+\delta-\bar{a}$, plus a peak of weight $(1-\alpha)$ at $a-\bar{a}$. Therefore,

$$q(\zeta) = \alpha\exp\,[2\pi i(1-\alpha)\delta\zeta]+(1-\alpha)\exp\,[-2\pi i\alpha\delta\zeta] \quad (6)$$

and

$$Q(\zeta) = \alpha\exp\,[2\pi i(a+\delta)\zeta]+(1-\alpha)\exp\,[2\pi ia\zeta]\,. \quad (7)$$

Hence

$$\begin{aligned}Q+Q^* &= 2(1-\alpha)\cos 2\pi a\zeta+2\alpha\cos 2\pi(a+\delta)\zeta\,, \\ QQ^* &= 1-4\alpha(1-\alpha)\sin^2 \pi\delta\zeta\,,\end{aligned}$$

and, therefore,

$$|G|^2 = \frac{4F^2K^2N_3\alpha(1-\alpha)\sin^2 \pi\delta\zeta}{\begin{array}{c}4\sin^2 \pi a\zeta+2\alpha\,(\cos 2\pi a\zeta-\cos 2\pi(a+\delta)\zeta) \\ -4\alpha(1-\alpha)\sin^2 \pi\delta\zeta\end{array}}\,. \quad (8)$$

Since in practice $\alpha \ll 1$, we may write

$$|G|^2 = F^2\left(\frac{\sin N_1\pi\xi a}{\sin \pi\xi a}\frac{\sin N_2\pi\eta a}{\sin \pi\eta a}\right)^2\frac{N_3\alpha\sin^2 \pi\delta\zeta}{\sin^2 \pi\zeta a}\,. \quad (9)$$

Equation (9) represents spikes of intensity at those reciprocal-lattice points for which $F^2 \neq 0$, with intensity falling off approximately as the square of the distance from a reciprocal-lattice point, and with relative spike magnitudes 0, $\sin^2 \pi\delta/a$, $\sin^2 2\pi\delta/a$, etc. In this last respect our result agrees with that of Frank, who shows that $\delta/a = 0{\cdot}35$ gives fair agreement with observation.

To relate this result to an experimental situation, we consider Fig. 1. Reference to James (1948) will show that the flux of intensity when the reflecting sphere intercepts a spike as shown, is

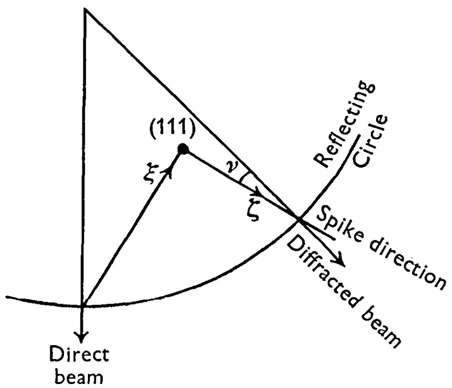

Fig. 1. Intersection of 'spike' by the reflecting circle.

$$J = J_0\left(\frac{e^2}{mc^2}\right)^2\frac{\lambda^2AB}{\cos\nu}\iint |G(\xi\eta\zeta)|^2d\xi d\eta\,, \quad (10)$$

where A allows for absorption of radiation in the crystal, B is the polarization factor, λ is the wavelength, ν is the angle shown in Fig. 1, and J_0 is the incident intensity per unit area.

Thus

$$J = J_0\left(\frac{e^2}{mc^2}\right)^2\frac{AB\lambda^2}{a^2\cos\nu}N_1N_2N_3F^2\frac{\alpha\sin^2 \pi\zeta\delta}{\pi^2R^2}\,. \quad (11)$$

We have written $\sin^2 \pi\zeta a \doteqdot (\pi R)^2$, where R is distance from a reciprocal-lattice point such that $\zeta =$

$(l+R)/a$. Introducing the crystal volume $V=N_1N_2N_3a^3$ and the unit-cell volume v, we have finally

$$J = J_0\left(\frac{e^2}{mc^2}\right)^2 \frac{ABa\lambda^2F^2V\alpha \sin^2 \pi\zeta\delta}{v^2\pi^2R^2 \cos \nu}\ . \qquad (12)$$

For a mosaic crystal rotated with angular velocity ω so that a reciprocal-lattice point passes through the reflecting sphere, the total energy reflected is

$$E = J_0\left(\frac{e^2}{mc^2}\right)^2 \frac{AB\lambda^3F^2V}{\omega v^2 \sin 2\theta}\ . \qquad (13)$$

From the ratio J/E the value of α can be found.

Finally in this section on theory we consider the effect of 'uneven-ness' in the abnormal spacing. The simplest model consists in having the displacement distributed normally about δ with standard deviation Δ. It is then readily shown from the general theory given above that the result corresponding to (7) is now

$$Q(\zeta) = \alpha \exp\left[-2\pi^2\Delta^2\zeta^2\right] \exp\left[2\pi i(a+\delta)\zeta\right] + (1-\alpha) \exp\left[2\pi i a\zeta\right]\ . \qquad (14)$$

The relative spike intensity varies as $1-QQ^*$, which in this case is approximately proportional to

$$1-\exp\left[-2\pi^2\Delta^2\zeta^2\right] \cos 2\pi\delta\zeta\ . \qquad (15)$$

By choosing appropriate values for δ and Δ one can fit the observed relative magnitudes only a little better than with the function $\sin^2 \pi\delta\zeta$. Equation (15) predicts that for large values of ζ (i.e. of the index l) the spikes become of equal magnitude. No measurements are available beyond $l = 5$; those beyond $l = 3$ rather suggest that the spike magnitude decreases to zero for large values of l.

3. Comparison with experiment

An octahedral diamond exhibiting strong spikes was set with [110] vertical, and the intensity of the spikes in the zero layer was measured at various distances R from (111), using a Geiger counter. The integrated intensity of the (111) reflexion was measured, but since it was suspected that this would be reduced by extinction, the integrated intensity of the (200) reflexion from a small crystal of LiH, known to be free from extinction, was also measured. Using subscripts D and L to denote the diamond and lithium hydride crystals respectively, we have, from (12) and (13),

$$\frac{J_D}{E_L} = \frac{a_D\alpha\omega \sin 2\theta \sin^2 \pi\zeta\delta}{\pi^2R^2\lambda \cos \nu} \frac{A_DB_DF_D^2V_Dv_L^2}{A_LB_LF_L^2V_Lv_D^2}\ . \qquad (16)$$

The following are the appropriate numerical values:

$a_D = 3{\cdot}57$ Å
$\lambda = 1{\cdot}54$ Å
$V_D = 0{\cdot}125$ mm.^{3}
$V_L = 0{\cdot}12$ mm.^{3}
$v_D = 46$ Å^3
$v_L = 68$ Å^3
$\omega = 0{\cdot}087$ rad.min.$^{-1}$

$F_D = 18{\cdot}0$
$F_L = 8{\cdot}7$
$A_D = 0{\cdot}45$
$A_L = 1{\cdot}0$
$B_D = B_L$
$\sin 2\theta = 0{\cdot}70$
$\cos \nu = 0{\cdot}97$

For $\delta/a = \frac{1}{3}$, $\sin^2 \pi\delta/a = 0{\cdot}75$. With foils to reduce the intensity by a factor 2^6, 800 counts were recorded per run of the LiH crystal through the reflecting position. This should be increased by 15% to allow for lost counts, giving $E_L = 5{\cdot}9\times10^4$ counts. Equation (14) then gives $\alpha \approx 3{\cdot}6\times10^{-4}JR^2$, where J is measured in counts per minute. This result is approximate in that the values of F^2 and of $\sin^2 \pi\zeta\delta$ have been taken to be constant and equal to their values at $\zeta = 1/a$ (or $R = 0$). In working out the values of α given in Table 1 a correction has been made for these factors, taking $\delta/a = \frac{1}{3}$. The variation of $\cos \nu$ is very little.

Values of J were recorded on a background of 370 counts min.$^{-1}$, so the standard deviation of α for the highest values of R is about 50%. Nevertheless, there is a possible lack of agreement with the theory for $|R| > 0{\cdot}1$. For smaller values of $|R|$, satisfactorily constant values of α are obtained, and we may take $\alpha = 1{\cdot}1\times10^{-3}$, with a standard deviation certainly less than 20%. (About half this value for α was given by

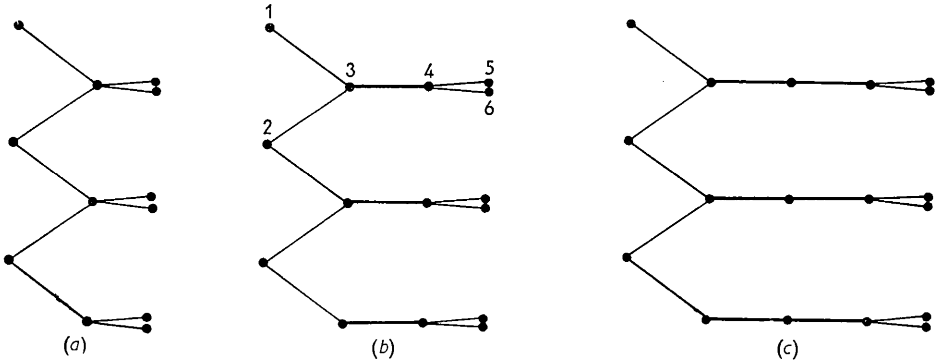

Fig. 2. (a) Normal arrangement of bonds in diamond. The two atoms shown as nearly coincident are respectively above and below the plane of the diagram. (b) Production of a displacement $0{\cdot}35a$ by introducing an extra layer of carbon atoms, with the formation of double bonds. (c) Production of a displacement $0{\cdot}7a$ by introducing two extra layers of carbon atoms.

Table 1

Value of R	J (counts min.$^{-1}$)	Relative value of F^2	Relative value of $\sin^2 \frac{1}{3}\pi(1+R)$	$\alpha \times 10^3$
−0·2	58	0·84	0·73	1·36
−0·18	93	0·87	0·76	1·64
−0·16	114	0·90	0·80	1·44
−0·14	131	0·93	0·83	1·20
−0·12	193	0·96	0·86	1·21
−0·10	263	0·98	0·89	1·12
−0·09	345	0·99	0·90	1·13
−0·08	452	0·99	0·91	1·15
−0·07	638	1·0	0·93	1·22
−0·06	854	1·0	0·94	1·18
−0·05	1230	1·0	0·95	1·16
−0·045	1475	1·0	0·96	1·12
0·0	—	1·00	1·00	—
0·045	1624	0·98	1·05	1·13
0·05	1329	0·97	1·06	1·18
0·06	811	0·95	1·07	1·03
0·07	558	0·93	1·09	0·97
0·08	502	0·92	1·10	1·14
0·09	385	0·90	1·11	1·14
0·10	284	0·87	1·12	1·05
0·12	135	0·83	1·13	0·82
0·14	117	0·78	1·15	0·92
0·16	85	0·75	1·17	0·90
0·18	42	0·72	1·18	0·58
0·20	43	0·67	1·20	0·77

us in an earlier report (Caticha-Ellis & Cochran, 1957); this was due to a mistake in calculation.)

Since faults in each of three directions are equally probable, but only one layer of atoms in four should be silicon to produce a unit cell of side $4a/3$, the atomic concentration of silicon required to give the above value of α is approximately 8×10^{-4}. The concentration of silicon in each of two diamonds exhibiting strong spikes did not exceed 10^{-5} (Lowde, private communication). In fact it seems unlikely that any impurity can be present in sufficient concentration to explain the spikes. It has been suggested by Dr A. R. Stokes (private communication) that the formation of double bonds between carbon atoms might be invoked to explain the spikes. Fig. 2(*a*) shows the arrangement of carbon atoms in a (110) plane. If an extra layer of carbon atoms is introduced as shown in Fig. 2(*b*) and the distance 3–4 is made 1·25 Å, a displacement $\delta = 0{\cdot}35a$ results. The arrangement is very unsatisfactory, since if C_3C_4 is a double bond, atoms 1...6 should be coplanar. This difficulty may be overcome by postulating the arrangement shown in Fig. 2(*c*), which gives $\delta = 0{\cdot}7a$, again taking the double-bond length as 1·25 Å, which is in any case rather short. This value of δ gives the same spike magnitudes, but the replacement of $\sin^2 \frac{1}{3}\pi(1+R)$ in column 4 of Table 1 by $\sin^2 \frac{2}{3}\pi(1+R)$ gives a greater spread of values of α. The arrangement is not plausible, and lacks confirmatory evidence, so we must conclude that we have no satisfactory physical explanation of the defects.

We would like to express our appreciation of the help we have had from Dr Grenville-Wells, and from Dr Kartha.

APPENDIX

We consider here the effect of allowing the displacement δ to occur between any of the four layers of atoms parallel to (001). Each layer is face-centred, and taking the origin of layer 0 to be at $(x, y) = (0, 0)$ the three subsequent layers at $z = \frac{1}{4}, \frac{1}{2}$ and $\frac{3}{4}$ respectively are related to layer 0 by translations to $(x, y) = (\frac{1}{4}, \frac{1}{4})$, $(0, \frac{1}{2})$ and $(-\frac{1}{4}, \frac{1}{4})$ respectively. For diamond, the systematic absences are those for a face-centred cubic lattice, but additional absences occur for $h+k+l = 4n+2$. For even indices $F = 8f$, for odd indices $F = 8f/\sqrt{2}$. This recapitulation is necessary in order to demonstrate that the defects do not produce spikes associated with points for which $F = 0$. Let F_n be the structure factor of the nth layer of atoms; it can assume four distinct values. Let d_n be the distance now of the nth layer along [001] from the crystal origin, and let $\bar{b} = \frac{1}{4}a+\beta\delta$ be the mean distance between layers. The probability of a fault per layer, β, is approximately $\frac{1}{4}\alpha$, since $\alpha \ll 1$. The number of layers is $4N_3$. We thus have

$$|G|^2 = K^2 \sum_0^{4N_3-1} F_n \exp\,[2\pi i\zeta d_n] \sum_0^{4N_3-1} F_n^* \exp\,[-2\pi i\zeta d_n]\,. \tag{A1}$$

Defining $q(\zeta)$ appropriately, i.e.

$$q(\zeta) = \exp\,[-2\pi i\beta\delta\zeta](\beta \exp\,[2\pi i\delta\zeta]+(1-\beta)) \tag{A2}$$

and

$$Q(\zeta) = q(\zeta) \exp\,[2\pi i\bar{b}\zeta]\,,$$

we find that

$$|G|^2 = 4K^2N_3\{A_0+A_1Q(\zeta)+A_2Q(\zeta)^2+\ldots \\ +A_1Q^*(\zeta)+A_2Q^*(\zeta)^2+\ldots\}\,, \tag{A3}$$

where

$$A_0 = \tfrac{1}{4}(F_0F_0^*+F_1F_1^*+F_2F_2^*+F_3F_3^*) = F_0^2\,,$$
$$A_1 = \tfrac{1}{4}(F_0^*F_1+F_1^*F_2+F_2^*F_3+F_3^*F_0)\,.$$

A_2 and A_3 are similarly defined, $A_4 = A_0$, $A_5 = A_1$, etc. Remembering that $F_1 = F_0 \exp\,[2\pi i(h+k)/4]$, etc., one finds there are four situations:

(i) $h+k$ odd: $F_0 = 0$; there is no intensity.
(ii) $h+k$ divisible by 4: $A_0 = A_1 = A_2 = A_3$.
(iii) h even, k even, but $h+k$ not divisible by 4: $A_1 = A_3 = -A_0$; $A_2 = A_0$.
(iv) h odd, k odd: $A_1 = A_3 = 0$; $A_2 = -A_0$.

For case (ii), the sums in (A3) can be evaluated as before, and we find eventually

$$|G|^2 = F_0^2 \frac{\sin^2 N_1\pi\xi a}{\sin^2 \pi\xi a} \frac{\sin^2 N_2\pi\eta a}{\sin^2 \pi\eta a} \frac{4N_3\beta \sin^2 \pi\zeta\delta}{\sin^2 (\pi\zeta a/4)}\,. \tag{A4}$$

It follows that there is a spike only when l is divisible by 4, and under (ii) this is also the condition for a Bragg reflexion. For such reflexions $F_0 = \frac{1}{4}F$, and, replacing $\sin\,(\pi\zeta a/4)$ by $\pi\zeta a/4$ and remembering that $\beta = \frac{1}{4}\alpha$, we see that (A4) reduces to the same result numerically as (9).

To find what happens when (iii) holds, we define

$$X(\delta, \zeta) = \sum_1^\infty q(\delta, \zeta)^n \exp\,[2\pi i n \bar{b} \zeta]\;.$$

Under condition (ii), therefore,

$$|G|^2 = 4K^2F_0^2N_3(1+X+X^*)\;,$$

whereas under condition (iii)

$$|G|^2 = 4K^2F_0^2N_3(1+Y+Y^*)\;,$$

where

$$Y(\delta, \zeta) = \sum_1^\infty (-1)^n q(\delta, \zeta)^n \exp\,[2\pi i \bar{b} \zeta]\;.$$

Put $\zeta' = \zeta + 1/2\bar{b}$ and define δ' so that $\delta\zeta = \delta'\zeta'$. We note that q is a function of the product $\delta\zeta$ (see (A2)).

Then

$$Y(\delta, \zeta) = \sum_1^\infty q(\delta', \zeta')^n \exp\,[2\pi i n \bar{b} \zeta'] = X(\delta', \zeta')\;.$$

The net result is that for $|G|^2$ under (iii), we have the same function as under (ii), but displaced by an amount $1/2\bar{b} \simeq 2/a$ in ζ, so that spikes occur only at $l = 2, 6, 10, \ldots$. Under (iii), those are the points for which Bragg reflexions occur. The spike magnitude is found to be as before.

A similar treatment applies to case (iv). It is found that the spike intensity $|G|^2$ is a factor 2 less than above; the spike magnitude is, however, the same since these are the reflexions for which F is a factor $\sqrt{2}$ less.

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The Crystal Structure of Diphenyltellurium Dibromide*

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Diphenyltellurium dibromide crystallizes with the space-group symmetry $I4_1$. There are four molecules of $(C_6H_5)_2TeBr_2$ in the unit cell for which $a = 11{\cdot}421 \pm 0{\cdot}010$ Å and $c = 9{\cdot}817 \pm 0{\cdot}010$ Å. The trial structure was determined by means of two-dimensional Patterson and Fourier syntheses and refined by means of three-dimensional Fourier syntheses and the least-squares routine on SWAC. The observed bond distances are $2{\cdot}682 \pm 0{\cdot}003$ Å for Te–Br and $2{\cdot}14 \pm 0{\cdot}03$ Å for Te–C, while the observed bond angles are $178{\cdot}0 \pm 0{\cdot}2°$ for Br–Te–Br and $96{\cdot}3 \pm 1{\cdot}2°$ for C–Te–C. Packing distances are all consistent with accepted van der Waals radii.

Introduction

X-ray diffraction studies of a number of diarylselenium dihalides have shown that the molecules of these substances involve nearly linear X–Se–X bonds with the Se–C bonds in a plane perpendicular to the axis of the halogen atoms (McCullough & Hamburger, 1941, 1942; McCullough & Marsh, 1950). An interesting feature of the structure is the observed selenium–halogen bonded distance, which is approximately 0·2 Å longer than the sum of the single covalent bond radii of the atoms involved (McCullough, 1953). By contrast, the observed selenium–carbon distance appears to be normal.

The investigation of structures of the type R_2TeX_2 is of interest, both as a natural extension of the above studies of selenium compounds and because of the general lack of detailed structural studies of compounds of tetracovalent tellurium. Preliminary X-ray diffraction studies of several compounds of the above type indicated that diphenyltellurium dibromide with only one-half molecule in the asymmetric unit was most promising.

Crystallographic data

Diphenyltellurium dibromide was prepared by Mr N. J. Krilanovich by the method of Krafft & Lyons (1894). The material was purified by recrystallization

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