consists of the spots due to the crystal of 6-layer structure and the continuous streak connecting these spots. It is found, however, that the streak is actually composed of a number of spots, due to the new modification, separated from each other by an equal short distance, about 0·3 mm. on the film taken in a camera of radius 8 cm. with Cu $K\alpha$ radiation, and we can enumerate 33 spots within the distance which corresponds to the c period of SiC(6). This observation shows that the reciprocal-lattice points of the new modification are distributed on the $(10\bar{1}l)$ rod with an interval $\frac{1}{33}$ of that for SiC(6), indicating a lattice period along the c axis corresponding to *at least* $6 \times 33 = 198$ layers.

The fine structure of the reciprocal-lattice rod, as found above for the $(10\bar{1}l)$ rod, can also be confirmed by observations on Laue photographs, on which the Laue lines due to SiC(6) as well as those due to the new modification appear simultaneously. Figs. 2 and 3 (*a*) show such Laue patterns taken on cylindrical films ($R = 8$ cm.) with the incident X-ray beams nearly parallel to the c axis and perpendicular to the $[11\bar{2}0]$ and $[1\bar{1}00]$ axes respectively, the latter axes being set parallel to the axis of the cylindrical films. Besides the intense Laue lines belonging to SiC(6) (denoted by $L(10\bar{1}1)(6)$, $L(10\bar{1}2)(6)$, etc.), there are regular line groups with moderate intensities which correspond to the new modification (denoted by s_n, $n = 0, 1, 2, \ldots$). We found just 33 lines of this kind between two Laue lines of SiC(6), say $L(10\bar{1}1)(6)$ and $L(10\bar{1}2)(6)$. The appearance of these s_n lines is explained on assuming for these reciprocal-lattice rods the same structure as deduced from the oscillation photograph, with due regard to the effect of higher harmonics. The Laue photographs, however, reveal more clearly that none of the reciprocal points of the new modification coincides with those of SiC(6) which have hexagonal symmetry. As is obvious from Fig. 3 (*b*), the reciprocal points of the latter structure are situated at a position one-third the way between the nearest two reciprocal-lattice points of the new modification. This one-third deviation is not a result of considerations arising from some trivial origins, since, as we have confirmed, it takes place for six rods $(10\bar{1}l)$, $(1\bar{1}0l)$, $(0\bar{1}1l)$, $(\bar{1}01l)$, $(\bar{1}10l)$ and $(01\bar{1}l)$ in common, but by changing the sense alternately, so that the distribution of the reciprocal points, as a whole, manifests the rhombohedral symmetry of the structure. The ultimate c period of the new modification, therefore, does not correspond to the above-mentioned $6 \times 33 = 198$ layers, but the triple of it, that is to say, $3 \times 6 \times 33 = 594$ layers. The factor 3, together with the one-third deviation of s_n-line group relative to SiC(6) Laue lines, is understood by the extinction rule of reflexions for the rhombohedral lattice.

The lattice period along the hexagonal c axis of the new modification is $2{\cdot}51 \times 594 \approx 1500$ A. The range of the ordering force for layers in this structure, therefore, should be at least $2{\cdot}51 \times 594 \div 3 \approx 500$ A., which cannot be understood in terms of the conventional type of force between layers.

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Largest likely values for the reliability index.

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The reliability index

$$R \equiv (\Sigma \,||\, F_{\text{obs.}} \,| - |\, F_{\text{calc.}} \,||)/(\Sigma \,|\, F_{\text{obs.}} \,|)$$

is widely used as a test of the quality of a structure determination. Values of R for trial structures are not often published, but it would seem that a structure giving R in the range 0·3–0·5 is accepted as showing promise of refinement. Dunitz (1949) gives 0·37 for his trial structure for 1,2,3,4-tetraphenylcyclobutane. Completed structure determinations usually have R less than 0·25, though higher values have been reported; Fenimore (1948) gives $R = 0{\cdot}31$–$0{\cdot}36$ and Geller & Hoard (1950) give 0·32. It seems of some interest to find the probable value of R for an entirely wrong structure, that is, one with the same symmetry as the correct structure, but with an unrelated arrangement of the same atoms.

Let F_1, F_2 be the values of $|\, F_{hkl} \,|$ for the two structures, X be $|\, F_1 - F_2 \,|$, and M be the number of reflexions on which R is to be based. Then

$$\begin{aligned} R &= M\langle X \rangle / M\langle |\, F \,| \rangle \\ &= \langle X \rangle / \langle |\, F \,| \rangle, \end{aligned} \tag{1}$$

where the angle brackets indicate average values. Since F_1 and F_2 are due to structures with the same symmetry and atoms, the probability, $P(F)\,dF$, that F lies between F and $F + dF$ is the same for both F_1 and F_2 (Wilson, 1949, 1950). A particular value of X can arise in two ways: (i) a value of F_1 may be paired with the value $F_2 = F_1 + X$, and (ii) a value of $F_1 > X$ may be paired with the value $F_2 = F_1 - X$. The probability, $Q(X)\,dX$, that X lies between X and $X + dX$ is therefore given by

$$\begin{aligned} Q(X) &= \int_0^\infty P(F)\,P(F+X)\,dF + \int_X^\infty P(F)\,P(F-X)\,dF \\ &= 2\int_0^\infty P(F)\,P(F+X)\,dF. \end{aligned} \tag{2}$$

Since $Q(X)$ is a probability-distribution function, a partial check of (2) is obtained by showing that the integral of $Q(X)$ from 0 to ∞ is unity, whatever the form of $P(F)$. For conciseness of expression in this and other manipulations below it is convenient first to introduce the functions $N(F)$ and $G(F)$ defined by the equations

$$\left.\begin{aligned} N(F) &\equiv \int_0^F P(F)\,dF, \\ dN(F) &= P(F)\,dF, \\ N(\infty) &= 1, \end{aligned}\right\} \tag{3}$$

$$\left.\begin{aligned} G(F) &\equiv \int_0^F FP(F)\,dF, \\ dG(F) &= FP(F)\,dF, \\ G(\infty) &= \langle |\, F \,| \rangle. \end{aligned}\right\} \tag{4}$$

Then

$$\int_0^\infty Q(X)\,dX = 2\int_0^\infty \left[\int_0^\infty P(F+X)\,dX\right] P(F)\,dF$$
$$= 2\int_0^\infty [1-N(F)]\,P(F)\,dF$$
$$= 2-\Big[N^2(F)\Big]_0^\infty = 1.$$

The mean value of X, required for evaluating R, is

$$\langle X\rangle = \int_0^\infty XQ(X)\,dX$$
$$= 2\int_0^\infty \left[\int_0^\infty XP(F+X)\,dX\right] P(F)\,dF$$
$$= 2\int_0^\infty [\langle|F|\rangle - G(F) - F + FN(F)]\,P(F)\,dF$$
$$= 2[\langle|F|\rangle - \langle G(F)\rangle - \langle|F|\rangle + G(\infty)\,N(\infty) - \langle G(F)\rangle]$$
$$= 2\langle|F|\rangle - 4\langle G(F)\rangle. \qquad (5)$$

The reliability index is therefore

$$R = 2 - 4\frac{\langle G(F)\rangle}{\langle|F|\rangle}. \qquad (6)$$

Since $G(F)$ is necessarily positive, $R<2$ whatever the probability distribution of the structure amplitudes.

For the usual centric and acentric distribution functions $\langle G(F)\rangle$ can be evaluated in terms of Σ, the average value of $|F|^2$ (Wilson, 1949), and more precise numerical values can be assigned to the probable value of R.

In the centric case

$$(\bar{1})\ G(F) = \left(\frac{2}{\pi\Sigma}\right)^{\frac{1}{2}}\int_0^F F\exp\{-F^2/2\Sigma\}\,dF$$
$$= \left(\frac{2\Sigma}{\pi}\right)^{\frac{1}{2}}[1-\exp\{-F^2/2\Sigma\}],$$
$$\langle G(F)\rangle = \frac{2}{\pi}\int_0^\infty [1-\exp\{-F^2/2\Sigma\}]\exp\{-F^2/2\Sigma\}\,dF$$
$$= \left(\frac{\Sigma}{\pi}\right)^{\frac{1}{2}}[\sqrt{2}-1], \qquad (7)$$

$$(\bar{1})\ R = 2\sqrt{2}-2 \doteq 0{\cdot}828, \qquad (8)$$

since $\langle F\rangle = (2\Sigma/\pi)^{\frac{1}{2}}$.

In the acentric case

$$(1)\ G(F) = 2\Sigma^{-1}\int_0^F F^2\exp\{-F^2/\Sigma\}\,dF$$
$$= -F\exp\{-F^2/\Sigma\} + \tfrac{1}{2}(\pi\Sigma)^{\frac{1}{2}}\operatorname{erf}(F/\Sigma^{\frac{1}{2}}),$$
$$\langle G(F)\rangle = -2\Sigma^{-1}\int_0^\infty F^2\exp\{-2F^2/\Sigma\}\,dF$$
$$+\left(\frac{\pi}{\Sigma}\right)^{\frac{1}{2}}\int_0^\infty F\operatorname{erf}(F/\Sigma^{\frac{1}{2}})\exp\{-F^2/\Sigma\}\,dF,$$

which gives, on integration by parts,

$$\langle G(F)\rangle = \left(\frac{\pi\Sigma}{32}\right)^{\frac{1}{2}}. \qquad (9)$$

The value of R is therefore

$$(1)\ R = 2-\sqrt{2} \doteq 0{\cdot}586, \qquad (10)$$

since $\langle|F|\rangle = \frac{1}{2}(\pi\Sigma)^{\frac{1}{2}}$. Thus R for an entirely wrong centrosymmetric structure is $\sqrt{2}$ times as big as for a wrong non-centrosymmetric structure.

Opinions of crystallographers differ whether 0·586 and 0·828 are surprisingly small or about what would be expected for entirely incorrect structures, but the former view appears to be the more prevalent. Certainly it seems that even correct non-centrosymmetric structures and projections will give inherently lower values of R than centrosymmetric, merely because of the lower dispersion of the acentric distribution function. It is therefore necessary to achieve a greater measure of agreement between observed and calculated F's before a non-centrosymmetric structure can be regarded as established.

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Reliability index for centrosymmetric and non-centrosymmetric structures.

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In a discussion of the value of the reliability index for wrong structures (Wilson, 1950), it was suggested that R is inherently higher for reflexions with a centric distribution, even when the structure is nearly correct, merely because of the higher dispersion of the distribution function. Two other properties of the centric distribution tend in the same direction: the smaller value of $\langle|F|\rangle$, and the larger proportion of weak reflexions (and therefore ordinarily the larger proportion of accidental absences). The former reduces the denominator of R and the latter acts mainly by increasing the numerator, though it has a smaller effect on the denominator as well.

For simplicity R will be calculated for a group of reflexions with approximately the same value of $\sin\theta/\lambda$, so that variation of the f's and the temperature factor can be neglected. The variation of R with $\sin\theta/\lambda$ is mentioned briefly below. The effect of $\langle|F|\rangle$ on the denominator is then simple; $\langle|F|\rangle = 0{\cdot}798\Sigma^{\frac{1}{2}}$ for centric distributions and $0{\cdot}887\Sigma^{\frac{1}{2}}$ for acentric (Wilson, 1949). Other things being equal, therefore, R for centrosymmetric structures or projections will be about 10 % of its value larger than for non-centrosymmetric structures or projections.

The effect of accidentally absent reflexions is a little more complicated. If the photographic techniques are