$1^{c} = 2\pi$ radians (Donnay & Donnay, 1949). We want to calculate

$$A_H = \sum_{n=1}^{N} f_n \cos HX_n \quad \text{and} \quad B_H = \sum_{n=1}^{N} f_n \sin HX_n .$$

For each of the N atoms in the cell, one card is prepared in which are hand-punched: a number j identifying the kind of atom, the running index n, and the co-ordinate X_n of the atom. This master set of N cards is reproduced as many times as there are reflections and, simultaneously, each set has its H value with corresponding $(\sin\theta)/\lambda$ (rounded off to 0·005) gang-punched into it. Then H is multiplied by X_n on the calculating punch (type 602) and the decimal part of the product, rounded off to three places, is punched into the data cards. Sort the cards on HX_n and merge with a set of one thousand 'function cards' that carry the values of α, $\sin\alpha$ and $\cos\alpha$, from $\alpha = 0{\cdot}000$ to $\alpha = 0{\cdot}999$ at intervals of 0·001 cycle. HX_n and α are used as control fields. By intersperse gang-punching the $\cos HX_n$ and $\sin HX_n$ values are transferred from the function cards on to the data cards. Sort on $(\sin\theta)/\lambda$ and on j, an operation which removes the function cards. Merge each of the j groups of data cards, on $(\sin\theta)/\lambda$ as control field, with the corresponding set of 'f_j cards'. These f_j cards are prepared once and for all; they carry $(\sin\theta)/\lambda$, j, and f_j for $(\sin\theta)/\lambda$ going from 0·000 to 1·500 at intervals of 0·005. The 602 punch is wired to multiply $\cos HX_n$ and $\sin HX_n$ by f_j and to punch the products into the data cards. Finally, sort on H or $(\sin\theta)/\lambda$, depending on the order in which the reflections are to be listed. The tabulator will print for each reflection: H, $(\sin\theta)/\lambda$, j, n, f_j, the contributions of each atom to A_H and B_H, as well as the sums A_H and B_H.

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Three new polymorphs of silicon carbide, 8*H*, 75*R*, and 84*R*.

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Three new polymorphs of silicon carbide have recently been discovered at the Mineralogical Laboratory, University of Michigan. The first of these has an eight-layered hexagonal unit cell, and is designated as type 8*H*. The crystal is an intergrowth of the new type with the more common 6*H*. Its structure has been established as having the zig-zag sequence 44 (Ramsdell, 1947). The second polymorph is rhombohedral and has a unit cell of 75 layers. The zig-zag sequence of type 75*R* is found to be 3232322323 (repeated three times). This structure was deduced by considering sequences involving only the numbers 2, 3 and 4, since no others have been observed in any of the known hexagonal or rhombohedral forms of silicon carbide.

The third polymorph is also rhombohedral and is an intergrowth with type 6*H*. On the basis of direct measurements on the Weissenberg photographs, it was not absolutely certain whether this new type is 81*R* or 84*R*. Using the same empirical limitation mentioned above, the only plausible solution seemed to be an 84-layered unit cell, with a zig-zag sequence of either 3333333232 or 3333323332 (each repeated three times). Intensity calculations have proved the first of these arrangements to be the correct one. The fact that the unit cell has 84 layers, rather than 81, was subsequently verified by the use of a Laue photograph, as suggested by Honjo, Miyake & Tomita (1950). In the Laue photograph, taken with a crystal-to-film distance of 6·5 cm., the resolution of the individual reflections is so much greater than on the Weissenberg films that there is no uncertainty in establishing the 84-layer character of this polymorph.

It will be noticed that neither of these two new rhombohedral types fits into the series proposed by Ramsdell (1947). This suggests the existence of a large number of additional polymorphs, the discovery of which may be effected by continued research. Several Weissenberg photographs obtained recently in our laboratory already indicate some new modifications.

In the near future the authors intend to describe, in a more detailed manner, these three new types of silicon carbide, and to discuss some structural implications of the ever-increasing number of polymorphs of this most unusual compound.

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Concerning reported discrepancies between X-ray and macroscopic measurements of thermal expansion of some alkali halides.

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A question of fundamental importance in the study of real crystals is the possibility of serious discrepancies in the values of those physical properties, such as thermal expansion, which may be studied by both X-ray and macroscopic means. Several measurements of the thermal expansion of metals using X-ray diffraction were made during the decade 1930–9, and for the most part the values agreed, within limits of experimental error, with the macroscopic values. The few cases of disagreement may have been due to the use of impure metals or to faulty temperature determination.

In a careful investigation on three alkali halides, however, Gott (1942) reported that the lattice expansion of pure potassium iodide, as measured by X-rays, was about 15% less than the macroscopic expansion in the range 20–190° C. A difference of this magnitude, if it exists, should result in such strains in the crystal as to produce obvious physical changes and would necessitate an extremely high degree of imperfection of the single crystal at elevated temperatures. As a possible explanation Gott suggested the difference between the surface layers of the crystal, which are effective in X-ray diffraction, and the internal structure of the crystal which results from Schottky false structure. In the Schottky picture, alkali and halogen ions leave their lattice positions and migrate to the surface of the crystal in numbers which increase with increased temperature. At the surface they take up new lattice positions, with the lattice points at the surface almost completely filled. However, the extent of this defect structure, which can be studied by a number of methods including electrical conductivity, alteration of density, and color-center phenomena, apparently is insufficient to produce differences of the magnitude observed by Gott.

Measurements have been made in this laboratory in an attempt to provide further information on this point. Two of the alkali halides reported on by Gott (KI and KBr) have been studied here. We are not able to support the discrepancy found by Gott; our values for the lattice-expansion coefficient show excellent agreement with the macroscopic values. Our measurements on both substances were made using two different types of high-temperature cameras, using two indirect and one direct method of temperature determination. One camera, a cylindrical powder camera with an electrically-heated furnace, has been described previously (Connell, 1947). In its use temperatures were measured both by calibration of the furnace, using known polymorphic transition points, and by the same standard-substance-admixture method used by Gott. The other camera consisted of a back-reflection cassette and pinhole system from a General Electric XRD unit and a simple liquid-bath furnace with a blade heater which was shown by test to provide direct temperature control of the powder sample.

Our measurements on KI were made using Fe $K\alpha$ radiation, instead of Cu $K\alpha$ as used by Gott, because of the superior back-reflection lines obtained with iron radiation. Two sets of back lines are produced, the (640) α_1 line at about 81° Bragg angle, and the (711) (551) α_1 line at 78° at room temperature. Measurements of the α_1 and α_2 lines from both sets of planes gave four sensitive back-region lines for measurement. KI samples were prepared from C. P. Baker's Analyzed KI of purity greater than 99·95%.

Lattice expansion of KBr was measured using both iron and copper radiations. With Fe $K\alpha_1$ radiation the (622) line falls at about 77° at room temperature, and with Cu $K\alpha_1$ the (660) (822) line falls at about 82°. The KBr was C. P. Baker's Analyzed, purity 99·99%.

The average expansion coefficients determined by us, together with the values calculated from Gott's results, are shown in Table 1. Our values represent an average of the results from diffraction patterns taken in both cameras. These results differed by less than 1%, but because of possible systematic error in the reading of the rather broad back-reflection lines, we estimate 2% as the probable accuracy of these values. The values shown for Gott's results are calculated from a curve plotted from his published data.

Table 1. *Average thermal expansion coefficients for* KI *and* KBr

Substance	Temp. range (° C.)	Our X-ray value ($\times 10^{-6}$)	Gott X-ray value ($\times 10^{-6}$)	Gott macroscopic value ($\times 10^{-6}$)
KI	20–100	40·6	37·2	40·8
	20–190	42·1	36·1	42·7
KBr	18–100	40·5	38·8	40·8
	18–190	41·7	40·5	41·4

It is seen that our values are in rather close agreement with Gott's macroscopic values and the difference between them is less than the combined limits of error.

Because of uncertainty in the interpretation of their results, we have not included in Table 1 the values reported by Eucken & Dannohl (1934) for the macroscopic expansion of these two substances. They do not define their 'true' expansion coefficient, but apparently mean $dl/l_{20}dt$ rather than $dl/l_t dt$. In either case we are unable to agree with Gott's interpretation of their results as agreeing closely with his own macroscopic values. Since it thus appears that there may be disagreement as to macroscopic expansivity also, we plan to make further measurements of both macroscopic and lattice expansion on the same crystalline sample.

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A preliminary X-ray investigation of dodecahydrotriphenylene, $C_{18}H_{24}$, and perhydrocoronene, $C_{24}H_{36}$.

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In the course of an extended research program on hydrogenated aromatic hydrocarbons with high molecular symmetry, the following structural data have so far been obtained: