We are grateful to Dr Perutz and our colleagues and visitors at this Unit, both for access to their data prior to publication and for helpful discussion of the problems involved. One of us (D. M. B.) is indebted to the Medical Research Council for a scholarship.

References

Blow, D. M. (1958). *Proc. Roy. Soc.* A, **247**, 302.
Bragg, W. L. & Perutz, M. F. (1954). *Proc. Roy. Soc.* A, **225**, 315.
Cramèr, H. (1937). *Random Variables and Probability Distributions.* Cambridge: Cambridge University Press.
Crick, F. H. C. & Magdoff, B. (1956). *Acta Cryst.* **9**, 901.
Cruickshank, D. W. J. (1959). *Acta Cryst.* **2**, 65.
Cullis, A. F., Dintzis, H. M. & Perutz, M. F. (1957). *Conference on Haemoglobin*, p. 50. (National Academy of Sciences, Washington, 1958).
Harker, D. (1956). *Acta Cryst.* **9**, 1.
Kendrew, J. C., Bodo, G., Dintzis, H. M., Parrish, R. G., Wyckoff, H. & Phillips, D. C. (1958). *Nature, Lond.* **181**, 662.
Perutz, M. F. (1956). *Acta Cryst.* **9**, 867.

Acta Cryst. (1959). **12**, 802

A Unified Program for Phase Determination, Type $3P_1$

By H. Hauptman and J. Karle

U.S. Naval Research Laboratory, Washington 25, D.C. U.S.A.

(*Received 5 March* 1959)

The unified program for phase determination, valid for all the space groups and both the equal and unequal atom cases, is continued here. The present paper is concerned with the centrosymmetric space groups comprising type $3P_1$. A detailed procedure for phase determination is described for this type.

1. Introduction

This is the fourth in a series of papers concerned with a program for phase determination initiated by us (Karle & Hauptman, 1959, hereafter referred to as $1P$). The application of the new probability methods, based on the Miller indices as random variables, is made to the space groups of type $3P_1$, (Hauptman & Karle, 1953). This type consists of the eleven primitive centrosymmetric space groups in the hexagonal system. We present here a detailed procedure for phase determination which utilizes the same general formula and, at the same time, makes use of relationships among the structure factors characteristic of each space group.

2. Notation

The same notation as appears in $1P$ (1959) is employed here.

3. Phase determining formulas

3·1. *Basic formulas*

$$B_{2,0}:\ \mathscr{E}_{\mathbf{h}}'^2 = 1+\frac{4\pi\sigma_2^2}{2^{(p+q+2)/2}pq\,\Gamma\left(\frac{p+1}{2}\right)\Gamma\left(\frac{q+1}{2}\right)\sigma_4} \times\langle\lambda_{p\mathbf{k}}\lambda_{q(\mathbf{h}+\mathbf{k})}\rangle_{\mathbf{k}}+R_{2,0}\,. \quad (3\cdot1\cdot1)$$

$$B_{3,0}:\ \mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2} = \frac{(2\pi)^{3/2}\sigma_2^3}{2^{(p+q+r+3)/2}pqr\,\Gamma\left(\frac{p+1}{2}\right)\Gamma\left(\frac{q+1}{2}\right)\Gamma\left(\frac{r+1}{2}\right)\sigma_4^{3/2}} \times\langle\lambda_{p\mathbf{k}}\lambda_{q(\mathbf{h}_1+\mathbf{k})}\lambda_{r(\mathbf{h}_1+\mathbf{h}_2+\mathbf{k})}\rangle_{\mathbf{k}} -2\frac{\sigma_6}{\sigma_4^{3/2}}+\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'''_{\mathbf{h}_1}+\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_2}+\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_1+\mathbf{h}_2})+R_{3,0}\,. \quad (3\cdot1\cdot2)$$

3·2. *Integrated formulas*

$$I_{2,0}:\ \mathscr{E}_{\mathbf{h}}'^2 = 1+\frac{2\sigma_2^2}{C_1^2(t)\,\sigma_4}\langle A_{t\mathbf{k}}A_{t(\mathbf{h}+\mathbf{k})}\rangle_{\mathbf{k}}+R'_{2,0}\,. \quad (3\cdot2\cdot1)$$

$$I_{3,0}:\ \mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2} = \frac{\sigma_2^3}{C_1^3(t)\sigma_4^{3/2}}\langle A_{t\mathbf{k}}A_{t(\mathbf{h}_1+\mathbf{k})}A_{t(\mathbf{h}_1+\mathbf{h}_2+\mathbf{k})}\rangle_{\mathbf{k}}-2\frac{\sigma_6}{\sigma_4^{3/2}}+\frac{\sigma_8^{1/2}}{\sigma_4} \times(\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'''_{\mathbf{h}_1}+\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_2}+\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_1+\mathbf{h}_2})+R'_{3,0}\,. \quad (3\cdot2\cdot2)$$

In these formulas, p, q, r and t are restricted to be positive. Ordinarily they are given values in the range 2–4.

The remainder terms are given in the appendix § 6 and in $1P$ (1959). Equation (3·1·1) or (3·2·1) serves to determine the magnitudes of the structure factors $|\mathscr{E}'_{\mathbf{h}}|$ corresponding to the squared structure. By means of equation (3·1·2) or (3·2·2), the phases of these structure factors $\varphi'_{\mathbf{h}}$ may be determined. In the next section we describe in detail how these equations are to be used for the various space groups included in type $3P_1$, (Monograph I, Table 1, p. 14, 1953).

4. Phase determining procedure

It is assumed that the $|\mathscr{E}_{\mathbf{h}}|$ have been calculated from the observed intensities. From these, the $|\mathscr{E}'_{\mathbf{h}}|$ are obtained by applying (3·1·1) or (3·2·1). In fact it may be advantageous to compute the $|\mathscr{E}'_{\mathbf{h}}|$ over a range of reflections extending beyond that of the original set of observations. We are here concerned only with the larger $|\mathscr{E}'_{\mathbf{h}}|$ and it is the phases of these whose values are to be determined. In the application of (3·1·2) or (3·2·2), the values of some $|\mathscr{E}'''_{\mathbf{h}}|$ may be required. These may be estimated from the corresponding $|\mathscr{E}_{\mathbf{h}}|$ or $|\mathscr{E}'_{\mathbf{h}}|$, or calculated from (3·1·1) or (3·2·1) in which $\mathscr{E}$ is replaced by $\mathscr{E}'$ and $\mathscr{E}'$ by $\mathscr{E}'''$, given sufficient data.

In the phase determining procedures to be described, it will be seen that the first steps concern the application of (3·1·2) or (3·2·2) with choices of indices which take full advantage of the space group symmetry. The final step is in the form of a general application which is the same for all the space groups.

The specification of the origin is carried out in conformance with the seminvariant theory previously developed (Monograph I, 1953). It is the same for all space groups of a given type. Therefore, a single procedure for origin specification obtains for all the space groups included in this paper.

In type $3P_1$, the phases φ_{hkl}, which are structure seminvariants, are of the form $l \equiv 0 \pmod 2$. In other words l must be even. This means that once the functional form of the structure factor has been chosen, the values of these phases are uniquely determined by the intensities alone. It is of interest to note, in the procedures to follow, how a single equation, (3·1·2) or (3·2·2), used in conjunction with relationships among the structure factors, characteristic of the particular space group and the chosen functional form for the structure factor, does, in fact, lead to unique values for the structure seminvariants.

4·1. *Hexagonal system*

We are concerned here with the eleven conventionally primitive, centrosymmetric space groups of the hexagonal system. The special choices for $\mathbf{h}_1$ and $\mathbf{h}_2$, in addition to $\mathbf{h}_1=\mathbf{h}_2$, are shown in the first two rows of Tables 1, 2, 3 and 4. Table 1 refers to all eleven space groups and, for the two choices of $\mathbf{h}_1$ and $\mathbf{h}_2$, the coefficient of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ is always $+1$. Tables 2, 3 and 4 list the coefficients of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ for additional choices of $\mathbf{h}_1$ and $\mathbf{h}_2$ derived from the relations among the structure factors in the particular space groups. Note that $P6/mmm$, $P6/mcc$, $P6_3/mmc$ and $P6_3/mcm$ have entries in Tables 2, 3 and 4. By means of the first choices in Table 3, $\mathbf{h}_1=(h_1, \bar{h}+h_1, l)$ and $\mathbf{h}_2=(h+\bar{h}_1, \bar{h}_1, l)$, equation (3·1·2) or (3·2·2) yields the value of $\mathscr{E}'^2_{h_1,\bar{h}+h_1,l}\mathscr{E}'_{h\bar{h}2l}$ multiplied by the numerical coefficient given in the second column of Table 3.

Table 1. *The choice of* $\mathbf{h}_1$ *and* $\mathbf{h}_2$ *for the eleven space groups of type* $3P_1$ *which may be inserted into* (3·1·2) *in order to obtain* $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ *from which* $\varphi'_{\mathbf{h}}$ *may be inferred. In these cases the coefficient of* $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ *is* $+1$ *for all the space groups*

$\mathbf{h}_1$	$\frac{1}{3}(2h+k)$,	$\frac{1}{3}(\bar{h}+k)$,	l_1	$\bar{k}$,	$h+k$,	l
$\mathbf{h}_2$	$\frac{1}{3}(h+\bar{k})$,	$\frac{1}{3}(h+2k)$,	$\bar{l}_1$	$h+k$,	$\bar{h}$,	l
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	h,	k,	0	h,	k,	$2l$
Condition	$h\equiv k \pmod 3$					

For example, for $P\bar{3}c1$, the relationship $\mathscr{E}'_{hkl}=(-1)^l\mathscr{E}'_{\bar{k}\bar{h}l}$ following from the chosen functional form for the structure factor, gives rise to the entry $(-1)^l$ in column 2, Table 3, for $P\bar{3}c1$. In this way the value of the phase $\varphi'_{h\bar{h}2l}$ is obtained. Since h_1 may be chosen arbitrarily, $\varphi'_{h\bar{h}2l}$ may possibly be determined in many ways. As always, the computations are performed for the larger values of $|\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}|$. With regard to the remaining choices of $\mathbf{h}_1$ and $\mathbf{h}_2$ in Tables 1–4, h_1, k_1, and l_1 may be chosen arbitrarily, permitting the possible use of many combinations of $\mathbf{h}_1$ and $\mathbf{h}_2$ for obtaining the value of the particular phase, $\varphi'_{\mathbf{h}}$.

We note that the phases obtained from Tables 1–4 include both the general and special cases of phases which are seminvariants, φ'_{hkl} ($l \equiv 0 \pmod 2$)). By the use of these, it is possible to calculate the values of additional phases which are seminvariants. This is accomplished by choosing $\mathbf{h}_1$ and $\mathbf{h}_2$ such that $\varphi'_{\mathbf{h}_1}$ and $\varphi'_{\mathbf{h}_2}$ have already been determined from application of Tables 1–4. It is to be noted that (3·1·2) or (3·2·2) will then yield the value of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$ from which the value of $\varphi'_{\mathbf{h}_1+\mathbf{h}_2}$ may be obtained.

Table 2. *The coefficients of* $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ *given by the left side of* (3·1·2) *or* (3·2·2), *for selected values of* $\mathbf{h}_1$ *and* $\mathbf{h}_2$ *and for each of six space groups in type* $3P_1$.

$\mathbf{h}_1$	h_1, $h+2\bar{h}_1$, l_1	$k+2\bar{k}_1$, k_1, l_1	h_1, $\bar{h}+h_1$, l_1	h_1, $h+\bar{h}_1$, l	h_1, $\bar{h}$, l	$\bar{k}$, k_1, l
$\mathbf{h}_2$	$h+\bar{h}_1$, $\bar{h}+2h_1$, $\bar{l}_1$	$\bar{k}+2k_1$, $k+\bar{k}_1$, l_1	$h+\bar{h}_1$, $\bar{h}_1$, $\bar{l}_1$	$h+\bar{h}_1$, h_1, l	$h+\bar{h}_1$, $\bar{h}$, l	$\bar{k}$, $k+\bar{k}_1$, l
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	h, 0, 0	0, k, 0	h, $\bar{h}$, 0	h, h, $2l$	h, $2\bar{h}$, $2l$	$2\bar{k}$, k, $2l$
$P\bar{3}1m$ $P6/mmm$ $P6_3/mcm$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
$P\bar{3}1c$ $P6/mcc$ $P6_3/mmc$	$(-1)^{l_1}$	$(-1)^{l_1}$	$(-1)^{l_1}$	$(-1)^l$	$(-1)^l$	$(-1)^l$

Table 3. *The coefficients of* $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ *given by the left side of* (3·1·2) *or* (3·2·2), *for selected values of* $\mathbf{h}_1$ *and* $\mathbf{h}_2$ *and for each of six space groups in type* $3P_1$.

$\mathbf{h}_1$	$h_1,\ \bar{h}+h_1,\ l$	$\frac{1}{2}(h+\bar{k}_1), k_1,\ l$	$h_1,\ \frac{1}{2}(k+\bar{h}_1),\ l$	$h_1,\ h+\bar{h}_1,\ l_1$	$h_1,\ \bar{h},\ l_1$	$h,\ k_1,\ l_1$
$\mathbf{h}_2$	$h+\bar{h}_1,\ \bar{h}_1,\ l$	$\frac{1}{2}(h+k_1), \bar{k}_1,\ l$	$\bar{h}_1,\ \frac{1}{2}(k+h_1),\ l$	$h+\bar{h}_1,\ h_1,\ \bar{l}_1$	$h+\bar{h}_1,\ \bar{h},\ \bar{l}_1$	$h,\ \bar{h}+\bar{k}_1,\ \bar{l}_1$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$h,\ \bar{h},\ 2l$	$h,\ 0,\ 2l$	$0,\ k,\ 2l$	$h,\ h,\ 0$	$h,\ 2\bar{h},\ 0$	$2h,\ \bar{h},\ 0$
		$k_1\equiv h$ (mod 2)	$h_1\equiv k$ (mod 2)			
$P\bar{3}m1$ $P6/mmm$ $P6_3/mmc$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
$P\bar{3}c1$ $P6/mcc$ $P6_3/mcm$	$(-1)^l$	$(-1)^l$	$(-1)^l$	$(-1)^{l_1}$	$(-1)^{l_1}$	$(-1)^{l_1}$

Table 4. *The coefficients of* $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ *given by the left side of* (3·1·2) *or* (3·2·2), *for selected values of* $\mathbf{h}_1$ *and* $\mathbf{h}_2$ *and for each of six space groups in type* $3P_1$.

$\mathbf{h}_1$	$h_1,\ k_1,\ l$	$\frac{1}{3}(2h+k),\ \frac{1}{3}(\bar{h}+k),\ l$	$h,\ k,\ l_1$	$\bar{k},\ h+k,\ l_1$
$\mathbf{h}_2$	$\bar{h}_1,\ \bar{k}_1,\ l$	$\frac{1}{3}(h+\bar{k}),\ \frac{1}{3}(h+2k),\ l$	$h,\ k,\ \bar{l}_1$	$h+k,\ \bar{h},\ \bar{l}_1$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$0,\ 0,\ 2l$	$h,\ k,\ 2l$	$2h,\ 2k,\ 0$	$h,\ k,\ 0$
		$h\equiv k$(mod 3)		
$P6/m$ $P6/mmm$ $P6/mcc$	$+1$	$+1$	$+1$	$+1$
$P6_3/m$ $P6_3/mcm$ $P6_3/mmc$	$(-1)^l$	$(-1)^l$	$(-1)^{l_1}$	$(-1)^{l_1}$

For the purpose of specifying the origin, a linearly semi-independent phase φ'_α having large corresponding $|\mathscr{E}'|$, is chosen. The value (0 or π) of φ'_α is then specified arbitrarily, thus fixing the origin. Systematic application of equation (3·1·2) or (3·2·2) then permits the determination of the phases $\varphi'_{\mathbf{h}}$ of all the remaining $\mathscr{E}'_{\mathbf{h}}$ of interest, using previously determined or specified phases as necessary.

Any phase $\varphi'_{hku}(u\equiv \text{odd})$ is a linearly semi-independent phase. We recall that phases of the type φ'_{hkg} ($g\equiv$ even) may be obtained directly from the intensities before an origin specification has been made. Is is readily seen that, starting with a specified phase of the form φ'_{hku}, it is possible to find, ultimately, the value of any desired phase $\varphi'_{\mathbf{h}}$ by suitable choice of $\mathbf{h}_1$ and $\mathbf{h}_2$, where $\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$.

5. Concluding remarks

This paper should be read in conjunction with $1P$ (1959), in which the symbols are defined and general remarks are made which are applicable to all the space groups.

The phase determining procedures offer many ways to calculate the value of a particular phase. This feature, together with the fact that the calculation of the right sides of (3·1·2) and (3·2·2) should yield not only the sign of the left side, but also its magnitude, serves as a good internal consistency check as the phase determination proceeds.

6. Appendix

The correction terms for the formulas listed in § 3 are given here and in $1P$ (1959). As a general rule, for larger N, they make a very small contribution. In any specific instance, the investigator can judge their importance for himself.

We define:

$$\begin{aligned}{}_7R_{2,0}= &-\frac{2\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'''_{00 2l}+\mathscr{E}'''_{hk0}+\mathscr{E}'''_{h+2k,2\bar{h}+\bar{k},0})\\ &-\frac{4\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}-\frac{\sigma_4}{2\sigma_2^2}\\ &\times((p-2)(p-4)+(q-2)(q-4))\mathscr{E}'^2_{\mathbf{h}}\\ &+\frac{5\sigma_6}{\sigma_2\sigma_4}(p+q-4)+\frac{\sigma_4}{8\sigma_2^2}((p-2)(q-2)\\ &+2(p-2)(p-4)+2(q-2)(q-4))+\dots,\end{aligned}\qquad(6\cdot1)$$

$$\begin{aligned}{}_8R_{2,0}= &-\frac{\sigma_8^{1/2}}{\sigma_4}(5\mathscr{E}'''_{00 2l}+2\mathscr{E}'''_{hk0}+2\mathscr{E}'''_{h+2k,2\bar{h}+\bar{k},0}\\ &+\mathscr{E}'''_{h+\bar{k},h+\bar{k},0}+\mathscr{E}'''_{h+k,h+k,0}+\mathscr{E}'''_{2h+k,0,0}\\ &+\mathscr{E}'''_{0,h+2k,0}+\mathscr{E}'''_{2h,\bar{h},0}+\mathscr{E}'''_{k,2\bar{k},0})\\ &-\frac{10\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\ &-\frac{5\sigma_4}{4\sigma_2^2}((p-2)(p-4)+(q-2)(q-4))\mathscr{E}'^2_{\mathbf{h}}\\ &+\frac{20\sigma_6}{\sigma_2\sigma_4}(p+q-4)\\ &+\frac{5\sigma_4}{16\sigma_2^2}((p-2)(q-2)+2(p-2)(p-4)\\ &+2(q-2)(q-4))+\dots,\end{aligned}\qquad(6\cdot2)$$

$$\begin{aligned}{}_7R_{3,0}= &-\frac{\sigma_4^{1/2}}{4\sigma_2}((r-2)\mathscr{E}'^2_{\mathbf{h}_1}+(p-2)\mathscr{E}'^2_{\mathbf{h}_2}\\ &+(q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_1.\end{aligned}\qquad(6\cdot3)$$

where

$$\varrho_1 = -\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1}(2\mathscr{E}'''_{h_1,\,k_1,\,l_1+2l_2}+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2,+k_1+k_2,\,l_1}$$
$$+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_1}+\mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,h_2+k_1+2k_2,\,l_1}$$
$$+\mathscr{E}'''_{h_1+2h_2+k_2,\,\bar{h}_2+k_1+k_2,\,l_1})$$
$$-\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_2}(2\mathscr{E}'''_{h_2,\,k_2,\,2l_1+l_2}+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1+k_2,\,l_2}$$
$$+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,h_1+2k_1+k_2,\,l_2}$$
$$+\mathscr{E}'''_{2h_1+h_2+k_1,\,\bar{h}_1+k_1+k_2,\,l_2})$$
$$-\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}(2\mathscr{E}'''_{h_1+h_2,\,k_1+k_2,\,l_1+\bar{l}_2}$$
$$+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1+k_2,\,l_1+l_2}+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_1+l_2}$$
$$+\mathscr{E}'''_{h_2+k_1,\,\bar{h}_1+\bar{k}_1+k_2,\,l_1+l_2}+\mathscr{E}'''_{h_1+k_2,\,\bar{h}_2+k_1+\bar{k}_2,\,l_1+l_2}) \qquad (6\cdot4)$$

$$_8R_{3,0} = -\frac{5\sigma_4^{1/2}}{4\sigma_2}$$
$$\times((r-2)\mathscr{E}'^2_{\mathbf{h}_1}+(p-2)\mathscr{E}'^2_{\mathbf{h}_2}+(q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_2\,, \qquad (6\cdot5)$$

where

$$\varrho_2 = -\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1}(5\mathscr{E}'''_{h_1,\,k_1,\,l_1+2l_2}+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1+k_2,\,l_1}$$
$$+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_1}+\mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,h_2+k_1+2k_2,\,l_1}$$
$$+\mathscr{E}'''_{h_1+2h_2+k_2,\,\bar{h}_2+k_1+k_2.\,l_1}+\mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,h_2+\bar{k}_1+\bar{k}_2,\,l_1}$$
$$+\mathscr{E}'''_{h_1+h_2+k_2,\,h_2+k_1+k_2,\,l_1}+\mathscr{E}'''_{h_1+\bar{k}_2,\,k_1+2k_2,\,l_1}$$
$$+\mathscr{E}'''_{h_1+2h_2+k_2,\,k_1,\,l_1}+\mathscr{E}'''_{h_1,\,h_2+k_1+2k_2,\,l_1}+\mathscr{E}'''_{h_1+2h_2,\,\bar{h}_2+k_1,\,l_1})$$
$$-\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_2}(5\mathscr{E}'''_{h_2,\,k_2,\,2l_1+l_2}+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1+k_2,\,l_2}$$
$$+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,h_1+2k_1+k_2,\,l_2}$$
$$+\mathscr{E}'''_{2h_1+h_2+k_1,\,\bar{h}_1+k_1+k_2,\,l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,\bar{h}_1+k_1+k_2,\,l_2}$$
$$+\mathscr{E}'''_{h_1+k_1+k_2,\,h_1+h_2+k_1,\,l_2}+\mathscr{E}'''_{h_2+\bar{k}_1,\,2k_1+k_2,\,l_2}$$
$$+\mathscr{E}'''_{2h_1+h_2+k_1,\,k_2,\,l_2}+\mathscr{E}'''_{2h_1+h_2,\,\bar{h}_1+k_2,\,l_2}+\mathscr{E}'''_{h_2,\,h_1+2k_1+k_2,\,l_2})$$
$$-\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}(5\mathscr{E}'''_{h_1+h_2,\,k_1+k_2,\,l_1+\bar{l}_2}+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1+k_2,\,l_1+l_2}$$
$$+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_1+l_2}+\mathscr{E}'''_{h_2+k_1,\,\bar{h}_1+\bar{k}_1+k_2,\,l_1+l_2}$$
$$+\mathscr{E}'''_{h_1+k_2,\,\bar{h}_2+k_1+\bar{k}_2,\,l_1+l_2}+\mathscr{E}'''_{h_2+k_1,\,h_1+k_2,\,l_1+l_2}$$
$$+\mathscr{E}'''_{h_2+\bar{k}_1,\,\bar{h}_1+k_2,\,l_1+l_2}+\mathscr{E}'''_{h_1+h_2+k_1,\,\bar{k}_1+k_2,\,l_1+l_2}$$
$$+\mathscr{E}'''_{\bar{h}_1+h_2+\bar{k}_1,\,k_1+k_2,\,l_1+l_2}+\mathscr{E}'''_{\bar{h}_1+h_2,\,h_1+k_1+k_2.\,l_1+l_2}$$
$$+\mathscr{E}'''_{h_1+h_2,\,\bar{h}_1+\bar{k}_1+k_2,\,l_1+l_2})\,. \qquad (6\cdot6)$$

Next we define (where $C_n(t)$ is replaced by C_n):

$$_7R'_{2,0} = -\frac{2\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'''_{00\,2l}+\mathscr{E}'''_{hk0}+\mathscr{E}'''_{h+2k,\,2\bar{h}+\bar{k},\,0})$$
$$+\frac{8\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}$$
$$-\frac{\sigma_4}{C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}}-\frac{10\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2)$$
$$+\frac{\sigma_4}{8C_1^2\sigma_2^2}((2C_1-C_2)^2+4C_1(8C_1-6C_2+C_3))+\ldots, \qquad (6\cdot7)$$

$$_8R'_{2,0} = -\frac{\sigma_8^{1/2}}{\sigma_4}(5\mathscr{E}'''_{00\,2l}+2\mathscr{E}'''_{hk0}+2\mathscr{E}'''_{h+2k,\,2\bar{h}+\bar{k},\,0}$$
$$+\mathscr{E}'''_{h+\bar{k},\,h+\bar{k},\,0}+\mathscr{E}'''_{h+k,\,h+k,\,0}+\mathscr{E}'''_{2h+k,\,0,\,0}+\mathscr{E}'''_{0,\,h+2k,\,0}$$
$$+\mathscr{E}'''_{2h,\,\bar{h},\,0}+\mathscr{E}'''_{k,\,2\bar{k},\,0})+\frac{20\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}$$
$$-\frac{5\sigma_4}{2C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}}-\frac{40\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2)$$
$$+\frac{5\sigma_4}{16C_1^2\sigma_2^2}((2C_1-C_2)^2+4C_1(8C_1-6C_2+C_3))+\ldots, \qquad (6\cdot8)$$

$$_7R'_{3,0} = \frac{\sigma_4^{1/2}}{4C_1\sigma_2}(2C_1-C_2)(\mathscr{E}'^2_{\mathbf{h}_1}+\mathscr{E}'^2_{\mathbf{h}_2}+\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_1\,, \qquad (6\cdot9)$$

and

$$_8R'_{3,0} = \frac{5\sigma_4^{1/2}}{4C_1\sigma_2}(2C_1-C_2)(\mathscr{E}'^2_{\mathbf{h}_1}+\mathscr{E}'^2_{\mathbf{h}_2}+\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_2\,. \qquad (6\cdot10)$$

In order to summarize the relations among the correction terms for for the various space groups in type $3P1$, it is convenient to identify

$$R\equiv R^{(0)}\,, \qquad (6\cdot11)$$

$$R'\equiv R^{(1)}\,. \qquad (6\cdot12)$$

Thus, for space groups $P\bar{3}$, $P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$ and $P\bar{3}c1$

$$R^{(j)}_{i,0} = {_1R^{(j)}_{i,0}};\quad j=0,1;\quad i=2,3\,. \qquad (6\cdot13)$$

For space groups $P6/m$ and $P6_3/m$,

$$R^{(j)}_{i,0} = {_1R^{(j)}_{i,0}}+{_7R^{(j)}_{i,0}};\quad j=0,1;\quad i=2,3\,. \qquad (6\cdot14)$$

Finally, for space groups $P6/mmm$, $P6/mcc$, $P6_3/mcm$, $P6_3/mmc$,

$$R^{(j)}_{i,0} = {_1R^{(j)}_{i,0}}+{_8R^{(j)}_{i,0}};\quad j=0,1;\quad i=2,3\,. \qquad (6\cdot15)$$

Note that $_1R_{2,0}$, $_1R_{3,0}$, $_1R'_{2,0}$ and $_1R'_{3,0}$ are defined in 1P (1959).

The remainder terms in the basic formulas are especially simple for the special case $p=q=r=2$. For this case, the formulas reduce to those obtainable by the algebraic methods proposed by us (1957).

References

HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem.* I. The Centrosymmetric Crystal. A.C.A. Monograph No. 3. New York: Polycrystal Book Service.

HAUPTMAN, H. & KARLE, J. (1957). *Acta Cryst.* **10**, 267.

KARLE, J. & HAUPTMAN, H. (1957). *Acta Cryst.* **10**, 515.

KARLE, J. & HAUPTMAN, H. (1959). *Acta Cryst.* **12**, 404.