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A Unified Program for Phase Determination, Type $3P_3$

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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 $3P_3$. A detailed procedure for phase determination is described for this type.

1. Introduction

This is the sixth 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 $3P_3$ (Hauptman & Karle, 1959). This type consists of the six space groups, $I4/m$, $I4_1/a$, $I4/mmm$, $I4/mcm$, $I4_1/amd$ and $I4_1/acd$ of the tetragonal system. Although these space groups are conventionally body-centered, they are referred, in this paper, to the primitive unit cell defined in our paper on the seminvariants (Hauptman & Karle, 1959). Also listed in the latter paper is a set of coordinates for each space group. This is equivalent to choosing the functional form for the structure factor which is employed in the present paper. 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*

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

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

3·2. *Integrated formulas*

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

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

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 $3P_3$.

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 (3·1·2). 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 (Hauptman & Karle, 1953, 1959). 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 $3P_3$, the phases φ_{hkl}, which are structure seminvariants, are of the form $h+k\equiv 0 \pmod 2$. In other words $h+k$ 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. *Tetragonal system, I-centered*

We are concerned here with space groups, $I4/m$, $I4_1/a$, $I4/mmm$, $I4/mcm$, $I4_1/amd$ and $I4_1/acd$. 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 and 2. By means of the first choice in Table 1,

$$\mathbf{h}_1=(h_1,\, h+\bar{h}_1,\, l_1) \quad\text{and}\quad \mathbf{h}_2=(h+\bar{h}_1,\, h_1,\, \bar{h}+l_1)\,,$$

equation (3·1·2) or (3·2·2) yields the value of

$$\mathscr{E}'^2_{h_1,\,h+\bar{h}_1,\,l_1}\mathscr{E}'_{hh\bar{h}}$$

multiplied by the numerical coefficient given in the second column of Table 1. For example, for $I4_1/a$, the relationship $\mathscr{E}'_{hkl}=(-1)^{h+l}\mathscr{E}'_{k,\,h,\,\bar{h}+\bar{k}+\bar{l}}$, following from the chosen functional form for the structure factor, gives rise to the entry $(-1)^{h_1+l_1}$ in column 2, Table 1. In this way the value of the phase $\varphi'_{hh\bar{h}}$ is determined. Since h_1 may be chosen arbitrarily, $\varphi'_{hh\bar{h}}$ 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 and 2, 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 φ'_{hkl} obtained from Tables 1 and 2 are seminvariants, i.e. $h+k\equiv 0 \pmod 2$. By use of these, it is possible to calculate the values of additional seminvariant phases. This is illustrated by means of the entries in Table 3. We note that (3·1·2) or (3·2·2) yields the value of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$ where $\mathscr{E}'_{\mathbf{h}_1}$ and $\mathscr{E}'_{\mathbf{h}_2}$ are assumed to have been found from Table 1.

Table 1

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 $3P_3$. The notation $P(I4/m)$ refers to the primitive unit cell, instead of the conventionally centered one (cf. Hauptman & Karle, 1959)

$\mathbf{h}_1$	$h_1,\ h+\bar{h}_1,\ l_1$*	$h_1,\ \bar{h}+h_1,\ \frac{1}{2}(h+l)+\bar{h}_1$*	$h_1,\ \bar{h}+l+h_1,\ h+\bar{h}_1$	$\frac{1}{4}(3h+k+2l),\ \frac{1}{4}(\bar{h}+k+2\bar{l}),\ \frac{1}{4}(\bar{h}+k+2l)$
$\mathbf{h}_2$	$h+\bar{h}_1,\ h_1,\ \bar{h}+l_1$	$h+\bar{h}_1,\ \bar{h}_1,\ \frac{1}{2}(\bar{h}+l)+h_1$	$h+\bar{h}_1,\ \bar{l}+\bar{h}_1,\ \bar{h}+l+h_1$	$\frac{1}{4}(h+\bar{k}+2\bar{l}),\ \frac{1}{4}(h+3k+2l),\ \frac{1}{4}(h+\bar{k}+2l)$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$h,\ h,\ \bar{h}$	$h,\ \bar{h},\ l$ $h+l\equiv 0 \pmod 2$	$h,\ \bar{h},\ l$	$h,\ k,\ l$ $h-k\equiv 2l \pmod 4$
$P(I4/m)$ $P(I4/mmm)$ $P(I4/mcm)$	+1*	+1*	+1	+1
$P(I4_1/a)$ $P(I4_1/amd)$ $P(I4_1/acd)$	$(-1)^{h_1+l_1}$*	$(-1)^{\frac{1}{2}(h+l)}$*	$(-1)^{h+l+h_1}$	$(-1)^{\frac{1}{4}(h-k+2l)}$

* The entries in these columns are to undergo cyclic permutation for the space groups, $P(I4/mmm)$, $P(I4/mcm)$, $P(I4_1/amd)$ and $P(I4_1/acd)$.

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 four space groups in type $3P_3$

$\mathbf{h}_1$	$h_1,\ \bar{h}+h_1,\ l_1$	$h_1,\ h+\bar{h}_1,\ l$	$h_1,\ l+\bar{h}_1+2\bar{l}_1,\ l_1$	$h,\ k,\ l_1$
$\mathbf{h}_2$	$h+\bar{h}_1,\ \bar{h}_1,\ \bar{l}_1$	$h+\bar{h}_1,\ h_1,\ l$	$\bar{h}_1,\ \bar{l}+h_1+2l_1,\ l+\bar{l}_1$	$h,\ k,\ \bar{h}+\bar{k}+\bar{l}_1$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$h,\ \bar{h},\ 0$	$h,\ h,\ 2l$	$0,\ 0,\ l$	$2h,\ 2k,\ \bar{h}+\bar{k}$
$P(I4/mmm)$	+1	+1	+1	+1
$P(I4/mcm)$	$(-1)^h$	$(-1)^h$	$(-1)^l$	$(-1)^{h+k}$
$P(I4_1/amd)$	$(-1)^{l_1}$	$(-1)^l$	$(-1)^{l+h_1}$	$(-1)^k$
$P(I4_1/acd)$	$(-1)^{h+l_1}$	$(-1)^{h+l}$	$(-1)^{h_1}$	$(-1)^h$

Table 3

Selected values of $\mathbf{h}_1$ and $\mathbf{h}_2$ to be inserted into (3·1·2) or (3·2·2) in order to obtain the product $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$ from which the value of the phase φ'_{hkl} ($h \equiv k \pmod 2$), the general seminvariant phase, may be inferred. A knowledge of $\varphi'_{\mathbf{h}_1}$ and $\varphi'_{\mathbf{h}_2}$ is required and may be obtained by use of Table 1

$\mathbf{h}_1$	$\frac{1}{2}(h+k)$,	$\frac{1}{2}(h+k)$,	$\frac{1}{2}(\bar{h}+\bar{k})$	h_1,	h_1,	$\bar{h}_1$
$\mathbf{h}_2$	$\frac{1}{2}(h+\bar{k})$,	$\frac{1}{2}(\bar{h}+k)$,	$\frac{1}{2}(h+k)+l$	$h+\bar{h}_1$,	$k+\bar{h}_1$,	$l+h_1$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	h,	k,	l	h,	k,	l
Condition		$h \equiv k \pmod 2$			$h \equiv k \pmod 2$; $h_1 \equiv \frac{1}{2}(h-k)+l \pmod 2$	

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 of the type φ'_{ugl} or φ'_{gul} ($g \equiv$ even, $u \equiv$ odd) is a linearly semi-independent phase. We recall that phases of the type φ'_{ggl} and φ'_{uul} may be determined directly from the intensities before an origin specification has been made. It is readily seen that any phase is accessible, once the origin specification has been made. This follows from the fact that, starting with the specified phase and those of the form φ'_{ggl} and φ'_{uul}, it is possible to express an arbitrary vector $\mathbf{h}$ (whose components have any parity) in the form $\mathbf{h}_1+\mathbf{h}_2$, where $\varphi'_{\mathbf{h}_1}$ and $\varphi'_{\mathbf{h}_2}$ are known. For example, if we specify a φ'_{ugl}, $\varphi'_{\mathbf{h}}=\varphi'_{gul}$ is obtainable from suitable phases $\varphi'_{\mathbf{h}_1}=\varphi'_{ugl_1}$ and $\varphi'_{\mathbf{h}_2}=\varphi'_{uul_2}$, where $\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$.

5. Concluding remarks

This paper should be read in conjunction with 1*P* (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 1*P* (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:

$$
\begin{aligned}
{}_{14}R_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}\left(2\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,k+l}+\mathscr{E}'''_{h+k,\,h+k,\,\bar{h}+\bar{k}}\right)\\
&-\frac{2\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{\sigma_4}{4\sigma_2^2}\left((p-2)(p-4)+(q-2)(q-4)\right)\mathscr{E}'^2_{\mathbf{h}}\\
&+\frac{2\sigma_6}{\sigma_2\sigma_4}(p+q-4)\\
&+\frac{\sigma_4}{16\sigma_2^2}\left((p-2)(q-2)+2(p-2)(p-4)\right.\\
&\left.+2(q-2)(q-4)\right)+\ldots,
\end{aligned} \tag{6·1}
$$

$$
\begin{aligned}
{}_{15}R_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}\left(3\mathscr{E}'''_{h+k,\,h+k,\,\bar{h}+\bar{k}}+\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,h+l}\right.\\
&+\mathscr{E}'''_{\bar{k}+\bar{l},\,k+l,\,k+l}+\mathscr{E}'''_{0,\,0,\,h+k+2l}+\mathscr{E}'''_{0,\,0,\,\bar{h}+k}\\
&\left.+2\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,k+l}\right)-\frac{6\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{3\sigma_4}{4\sigma_2^2}\left((p-2)(p-4)+(q-2)(q-4)\right)\mathscr{E}'^2_{\mathbf{h}}\\
&+\frac{9\sigma_6}{\sigma_2\sigma_4}(p+q-4)\\
&+\frac{3\sigma_4}{16\sigma_2^2}\left((p-2)(q-2)+2(p-2)(p-4)\right.\\
&\left.+2(q-2)(q-4)\right)+\ldots,
\end{aligned} \tag{6·2}
$$

$$
\begin{aligned}
{}_{14}R_{3,0} = &-\frac{\sigma_4^{1/2}}{8\sigma_2}\left((r-2)\mathscr{E}'^2_{\mathbf{h}_1}+(p-2)\mathscr{E}'^2_{\mathbf{h}_2}\right.\\
&\left.+(q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2}\right)+\varrho_1,
\end{aligned} \tag{6·3}
$$

where,

$$
\begin{aligned}
\varrho_1 = &-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1}\left(\mathscr{E}'''_{h_1+h_2+k_2,\,h_2+k_1+k_2,\,\bar{h}_2+\bar{k}_2+l_1}\right.\\
&+\mathscr{E}'''_{h_1+h_2+l_2,\,\bar{h}_2+k_1+\bar{l}_2,\,k_2+l_1+l_2}\\
&\left.+\mathscr{E}'''_{h_1+\bar{k}_2+\bar{l}_2,\,k_1+k_2+l_2,\,h_2+l_1+l_2}\right)\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_2}\left(\mathscr{E}'''_{h_1+h_2+k_1,\,h_1+k_1+k_2,\,\bar{h}_1+\bar{k}_1+l_2}\right.\\
&+\mathscr{E}'''_{h_1+h_2+l_1,\,\bar{h}_1+k_2+\bar{l}_1,\,k_1+l_1+l_2}\\
&\left.+\mathscr{E}'''_{h_2+\bar{k}_1+\bar{l}_1,\,k_1+k_2+l_1,\,h_1+l_1+l_2}\right)\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\left(\mathscr{E}'''_{h_1+\bar{k}_2,\,\bar{h}_2+k_1,\,h_2+k_2+l_1+l_2}\right.\\
&+\mathscr{E}'''_{h_1+\bar{l}_2,\,h_2+k_1+k_2+l_2,\,\bar{k}_2+l_1}\\
&\left.+\mathscr{E}'''_{h_1+h_2+k_2+l_2,\,k_1+\bar{l}_2,\,\bar{h}_2+l_1}\right)+\ldots,
\end{aligned} \tag{6·4}
$$

and

$$
{}_{15}R_{3,0} = -\frac{3\sigma_4^{1/2}}{8\sigma_2}\big((r-2)\mathscr{E}'^2_{\mathbf{h}_1} + (p-2)\mathscr{E}'^2_{\mathbf{h}_2} + (q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2}\big) + \varrho_2\,, \qquad (6{\cdot}5)
$$

where,

$$
\begin{aligned}
\varrho_2 = {} & -\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1}\big(3\mathscr{E}'''_{h_1+h_2+k_2,\,h_2+k_1+k_2,\,\bar{h}_2+\bar{k}_2+l_1} \\
& + \mathscr{E}'''_{h_1+h_2+l_2,\,\bar{h}_2+k_1+\bar{l}_2,\,h_2+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+h_2+l_2,\,\bar{h}_2+k_1+\bar{l}_2,\,k_2+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+\bar{k}_2+\bar{l}_2,\,k_1+k_2+l_2,\,h_2+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+\bar{k}_2+\bar{l}_2,\,k_1+k_2+l_2,\,k_2+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,\bar{h}_2+k_1+k_2,\,l_1} + \mathscr{E}'''_{h_1,\,k_1,\,h_2+k_2+l_1+2l_2}\big) \\
& - \frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_2}\big(3\mathscr{E}'''_{h_1+h_2+k_1,\,h_1+k_1+k_2,\,\bar{h}_1+\bar{k}_1+l_2} \\
& + \mathscr{E}'''_{h_1+h_2+l_1,\,\bar{h}_1+k_2+\bar{l}_1,\,h_1+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+h_2+l_1,\,\bar{h}_1+k_2+\bar{l}_1,\,k_1+l_1+l_2} \\
& + \mathscr{E}'''_{h_2+\bar{k}_1+\bar{l}_1,\,k_1+k_2+l_1,\,h_1+l_1+l_2} \\
& + \mathscr{E}'''_{h_2+\bar{k}_1+\bar{l}_1,\,k_1+k_2+l_1,\,k_1+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,\bar{h}_1+k_1+k_2,\,l_2} + \mathscr{E}'''_{h_2,\,k_2,\,h_1+k_1+2l_1+l_2}\big) \\
& - \frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\big(3\mathscr{E}'''_{h_1+\bar{k}_2,\,\bar{h}_2+k_1,\,h_2+k_2+l_1+l_2} \\
& + \mathscr{E}'''_{h_1+\bar{l}_2,\,h_2+k_1+k_2+l_2,\,\bar{h}_2+l_1} + \mathscr{E}'''_{h_1+\bar{l}_2,\,h_2+k_1+k_2+l_2,\,\bar{k}_2+l_1} \\
& + \mathscr{E}'''_{h_1+h_2+k_2+l_2,\,k_1+\bar{l}_2,\,\bar{h}_2+l_1} + \mathscr{E}'''_{h_1+h_2+k_2+l_2,\,k_1+l_2,\,\bar{k}_2+l_1} \\
& + \mathscr{E}'''_{h_2+k_1,\,h_1+k_2,\,l_1+l_2} \\
& + \mathscr{E}'''_{h_1+h_2,\,k_1+k_2,\,\bar{h}_1+\bar{k}_1+\bar{l}_1+l_2}\big) + \dots\,, \qquad (6{\cdot}6)
\end{aligned}
$$

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

$$
\begin{aligned}
{}_{14}R'_{2,0} = {} & -\frac{\sigma_8^{1/2}}{\sigma_4}\big(2\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,k+l} + \mathscr{E}'''_{h+k,\,h+k,\,\bar{h}+\bar{k}}\big) \\
& + \frac{4\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}} \\
& - \frac{\sigma_4}{2C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}} - \frac{4\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2) \\
& + \frac{\sigma_4}{16C_1^2\sigma_2^2}\big((2C_1-C_2)^2 + 4C_1(8C_1 \\
& - 6C_2+C_3)\big) + \dots\,, \qquad (6{\cdot}7)
\end{aligned}
$$

$$
\begin{aligned}
{}_{15}R'_{2,0} = {} & -\frac{\sigma_8^{1/2}}{\sigma_4}\big(3\mathscr{E}'''_{h+k,\,h+k,\,\bar{h}+\bar{k}} + \mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,h+l} \\
& + \mathscr{E}'''_{\bar{k}+\bar{l},\,k+l,\,k+l} + \mathscr{E}'''_{0,\,0,\,h+k+2l} + \mathscr{E}'''_{0,\,0,\,\bar{h}+k} \\
& + 2\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,k+l}\big) + \frac{12\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}} \\
& - \frac{3\sigma_4}{2C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}} - \frac{18\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2) \\
& + \frac{3\sigma_4}{16C_1^2\sigma_2^2}\big((2C_1-C_2)^2 \\
& + 4C_1(8C_1-6C_2+C_3)\big) + \dots\,, \qquad (6{\cdot}8)
\end{aligned}
$$

$$
{}_{14}R'_{3,0} = \frac{\sigma_4^{1/2}}{8C_1\sigma_2}(2C_1-C_2)\big(\mathscr{E}'^2_{\mathbf{h}_1} + \mathscr{E}'^2_{\mathbf{h}_2} + \mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2}\big) + \varrho_1\,, \qquad (6{\cdot}9)
$$

and

$$
{}_{15}R'_{3,0} = \frac{3\sigma_4^{1/2}}{8C_1\sigma_2}(2C_1-C_2)\big(\mathscr{E}'^2_{\mathbf{h}_1} + \mathscr{E}'^2_{\mathbf{h}_2} + \mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2}\big) + \varrho_2\,. \qquad (6{\cdot}10)
$$

In order to summarize the relations among the correction terms for the various space groups in type $3P_3$, it is convenient to identify

$$
R \equiv R^{(0)}, \qquad (6{\cdot}11)
$$

$$
R' \equiv R^{(1)}. \qquad (6{\cdot}12)
$$

Thus, for space groups $I4/m$ and $I4_1/a$,

$$
R^{(j)}_{i,0} = {}_1R^{(j)}_{i,0} + {}_{14}R^{(j)}_{i,0}; \quad j=0,1; \quad i=2,3\,. \qquad (6{\cdot}13)
$$

For space groups $I4/mmm$, $I4/mcm$, $I4_1/amd$ and $I4_1/acd$,

$$
R^{(j)}_{i,0} = {}_1R^{(j)}_{i,0} + {}_{15}R^{(j)}_{i,0}; \quad j=0,1; \quad i=2,3\,. \qquad (6{\cdot}14)
$$

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).

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