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A Unified Program for Phase Determination, Type $2P_1$

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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 $2P_1$. A detailed procedure for phase determination is described for this type.

1. Introduction

This is the third in a series of papers 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 here to the space groups of type $2P_1$ (Hauptman & Karle, 1959). This type consists of the four space groups *Immm*, *Ibam*, *Imma* and *Ibca* of the orthorhombic system. Although these space groups are conventionally body-centered, they are referred, in this paper, to the primitive unit cell as 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. A detailed procedure for phase determination in the space groups of type $2P_1$ will be presented 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

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

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

3·2. Integrated formulas

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

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

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.

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 the $|\mathscr{E}'_{\mathbf{h}}|$ so computed may be made to cover 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). Origin specification in all space groups of a given type is the same. Thus, the specification for space group *Immm* serves as a model for the remaining ones of type $2P_1$.

In type $2P_1$, the phases φ_{hkl}, which are structure seminvariants, are of the form $h \equiv k \equiv l \pmod 2$. In other words h, k and l are either all odd or all even. This means that once the functional form for 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. *Orthorhombic system, I-centered*

We are concerned here with space groups *Immm*, *Ibam*, *Imma* and *Ibca*.* The six 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 Table 1. By means of the first of these choices, $\mathbf{h}_1 = (h_1, k_1, h+\bar{k}_1)$ and $\mathbf{h}_2 = (\bar{h}+\bar{h}_1, h+\bar{k}_1, k_1)$, equation (3·1·2) or (3·2·2) yields the value of $\mathscr{E}'^2_{h_1,k_1,h+\bar{k}_1}\mathscr{E}'_{\bar{h}hh}$ multiplied by the numerical coefficient given in the second column of Table 1. For example, for *Ibam*, the relationship $\mathscr{E}'_{hkl} = (-1)^{h+k}\mathscr{E}'_{h+k+l,\bar{l},\bar{k}}$ following from the chosen functional form for the structure factor, gives rise to the entry $(-1)^{h_1+k_1}$ in column 2, Table 1 for *Ibam*. In this way the value of the phase $\varphi'_{\bar{h}hh}$ is determined. Since h_1 and k_1 may be chosen arbitrarily, $\varphi'_{\bar{h}hh}$ may possibly be determined in many ways. As always, the computations are performed for the larger values of $|\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}|$.

The remaining choices for $\mathbf{h}_1$ and $\mathbf{h}_2$ of Table 1 yield, in a similar way, the values of $\varphi'_{h\bar{h}h}$, $\varphi'_{hh\bar{h}}$, $\varphi'_{hk\bar{k}}$, $\varphi'_{\bar{l}kl}$ and $\varphi'_{h\bar{h}l}$. The entries in this table are the coefficients of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ which occurs on the left side of (3·1·2) or (3·2·2). In general 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 a particular phase.

We note that the phases obtained from Table 1 are special cases of phases which are seminvariants. By the use of these, it is possible to calculate the values of phases of a general type which are seminvariants, $\varphi_{hkl}(h \equiv k \equiv l \pmod 2)$. This is accomplished by means of the entries in Table 2, in which φ_{hkl} is a general seminvariant. It is to be noted that (3·1·2) or (3·2·2) now 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 by use of Table 1. Again, h_1, k_1 and l_1 in columns 5, 6 and 7 of Table 2 are arbitrary, but limited by the set of previously determined phases.

For the purpose of specifying the origin, a linearly

* The discussion to follow is equally valid for the four supergroups included in Tables 1 and 2.

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 the four space groups comprising type $2P_1$. Four supergroups of type $3P_3$ are included for later reference. The notation $P(Immm)$ refers to the primitive unit cell, instead of the conventionally centered one (cf. Hauptman & Karle, 1959)

$\mathbf{h}_1$	$h_1,\ k_1,\ h+\bar{k}_1$	$h+\bar{l}_1,\ k_1,\ l_1$	$h_1,\ h+\bar{h}_1,\ l_1$	$h_1,\ \frac{1}{2}(h+k+2\bar{h}_1),\ \frac{1}{2}(h+\bar{k}+2\bar{h}_1)$	$\frac{1}{2}(k+\bar{l}+2\bar{k}_1),\ k_1,\ \frac{1}{2}(k+l+2\bar{k}_1)$	$\frac{1}{2}(h+l+2\bar{l}_1),\ \frac{1}{2}(\bar{h}+l+2\bar{l}_1),\ l_1$
$\mathbf{h}_2$	$\bar{h}+\bar{h}_1,\ h+\bar{k}_1,\ k_1$	$l_1,\ \bar{h}+\bar{k}_1,\ h+\bar{l}_1$	$h+\bar{h}_1,\ h_1,\ \bar{h}+l_1$	$h+\bar{h}_1,\ \frac{1}{2}(\bar{h}+k+2h_1),\ \frac{1}{2}(\bar{h}+\bar{k}+2h_1)$	$\frac{1}{2}(\bar{k}+\bar{l}+2k_1),\ k+\bar{k}_1,\ \frac{1}{2}(\bar{k}+l+2k_1)$	$\frac{1}{2}(h+\bar{l}+2l_1),\ \frac{1}{2}(\bar{h}+\bar{l}+2l_1),\ l+\bar{l}_1$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$\bar{h},\ h,\ h$	$h,\ \bar{h},\ h$	$h,\ h,\ \bar{h}$	$h,\ k,\ \bar{k}$	$\bar{l},\ k,\ l$	$h,\ \bar{h},\ l$
				$h \equiv k \pmod 2$	$k \equiv l \pmod 2$	$h \equiv l \pmod 2$
$P(Immm)$ $P(I4/mmm)$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
$P(Ibam)$ $P(I4/mcm)$	$(-1)^{h_1+k_1}$	$(-1)^{h+k_1+l_1}$	$+1$	$(-1)^{\frac{1}{2}(h+k)}$	$(-1)^{\frac{1}{2}(k-l)}$	$+1$
$P(Imma)$ $P(I4_1/amd)$	$+1$	$(-1)^{h}$	$(-1)^{h_1+l_1}$	$+1$	$(-1)^{k}$	$(-1)^{\frac{1}{2}(h+l)}$
$P(Ibca)$ $P(I4_1/acd)$	$(-1)^{h_1+k_1}$	$(-1)^{k_1+l_1}$	$(-1)^{h_1+l_1}$	$(-1)^{\frac{1}{2}(h+k)}$	$(-1)^{\frac{1}{2}(k+l)}$	$(-1)^{\frac{1}{2}(h+l)}$

Table 2

A list 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 $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}}$ from which the value of the phase φ'_{hkl} $(h \equiv k \equiv l \pmod 2)$, the general seminvariant phase, may be inferred. This requires a knowledge of $\varphi'_{\mathbf{h}_1}$ and $\varphi'_{\mathbf{h}_2}$ which may be obtained by use of Table 1. Thus, this list has a particular significance for the eight space groups included in Table 1.

$\mathbf{h}_1$	$\frac{1}{2}(\bar{k}+\bar{l})$,	$\frac{1}{2}(k+\bar{l})$,	$\frac{1}{2}(k+l)$	$\frac{1}{2}(h+l)$,	$\frac{1}{2}(\bar{h}+\bar{l})$,	$\frac{1}{2}(h+l)$	$\frac{1}{2}(h+k)$,	$\frac{1}{2}(h+k)$,	$\frac{1}{2}(\bar{h}+\bar{k})$	h_1,	$\bar{h}_1$,	$k+l+h_1$	$h+l+k_1$,	k_1,	$\bar{k}_1$	$\bar{l}_1$,	$h+k+l_1$,	l_1
$\mathbf{h}_2$	$h+\frac{1}{2}(k+l)$,	$\frac{1}{2}(k+\bar{l})$,	$\frac{1}{2}(\bar{k}+l)$	$\frac{1}{2}(h+\bar{l})$,	$k+\frac{1}{2}(h+l)$,	$\frac{1}{2}(\bar{h}+l)$	$\frac{1}{2}(h+\bar{k})$,	$\frac{1}{2}(\bar{h}+k)$,	$l+\frac{1}{2}(h+k)$	$h+\bar{h}_1$,	$k+h_1$,	$\bar{k}+\bar{h}_1$	$\bar{l}+\bar{k}_1$,	$k+\bar{k}_1$,	$l+k_1$	$h+l_1$,	$\bar{h}+\bar{l}_1$,	$l+\bar{l}_1$
$\mathbf{h} = \mathbf{h}_1+\mathbf{h}_2$	h,	k,	l	h,	k,	l	h,	k,	l	h,	k,	l	h,	k,	l	h,	k,	l

semi-independent pair of phases φ'_α and φ'_β, having large corresponding $|\mathscr{E}'|$, is chosen. The values (0 or π) of φ'_α and φ'_β are 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.

An example of a linearly semi-independent pair of phases is φ'_{ggu} and φ'_{gug} ($g \equiv$ even, $u \equiv$ odd). We recall that phases of the type φ'_{ggg} and φ'_{uuu} may be obtained directly from the intensities before an origin specification has been made. Additional phases are obtainable from these by suitable choice of $\mathbf{h}_1$ and $\mathbf{h}_2$ in (3·1·2) or (3·2·2). 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 phases and those of the form φ'_{ggg} and φ'_{uuu}, 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, $\varphi'_{\mathbf{h}} = \varphi'_{uug}$ is obtainable from suitable phases $\varphi'_{\mathbf{h}_1} = \varphi'_{uuu}$ and $\varphi'_{\mathbf{h}_2} = \varphi'_{ggu}$, where $\mathbf{h} = \mathbf{h}_1+\mathbf{h}_2$. Again, $\varphi'_{\mathbf{h}} = \varphi'_{ugg}$ is obtainable from suitable phases $\varphi'_{\mathbf{h}_1} = \varphi'_{uug}$ and $\varphi'_{\mathbf{h}_2} = \varphi'_{gug}$, where $\mathbf{h} = \mathbf{h}_1+\mathbf{h}_2$. The remaining types *ugu* and *guu* are similarly obtained.

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.

Tables 1 and 2 contain the main choices of interest among $\mathbf{h}_1$, $\mathbf{h}_2$ and $\mathbf{h} = \mathbf{h}_1+\mathbf{h}_2$ for space groups of type $2P_1$. In addition, these choices are also valid for four of the supergroups of type $3P_3$, to be treated further in a subsequent paper.

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.

The calculation of an $\mathscr{E}'^2$ map, in the case of unequal atoms, may be a particularly useful adjunct to the procedure, since it exaggerates the Patterson peaks arising from the heaviest atoms.

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, these terms make a very small contribution. In any specific instance, the investigator can judge their importance for himself.

We define:

$$
\begin{aligned}
{}_6R_{2,\,0} = {} & -\frac{\sigma_8^{1/2}}{\sigma_4}\left(\mathscr{E}'''_{h+k,\,h+k,\,\bar{h}+\bar{k}}+\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,h+l}+\mathscr{E}'''_{\bar{k}+\bar{l},\,k+l,\,k+l}\right) \\
& -\frac{2\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\,\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}-\frac{\sigma_4}{4\sigma_2^2} \\
& \qquad \times\left((p-2)(p-4)+(q-2)(q-4)\right)\mathscr{E}'^{2}_{\mathbf{h}} \\
& +\frac{2\sigma_6}{\sigma_2\sigma_4}(p+q-4)+\frac{\sigma_4}{16\sigma_2^2}\left((p-2)(q-2)\right. \\
& \left.+2(p-2)(p-4)+2(q-2)(q-4)\right)+\ldots\,, \qquad (6{\cdot}1)
\end{aligned}
$$

$$
\begin{aligned}
{}_6R_{3,\,0} = {} & -\frac{\sigma_4^{1/2}}{8\sigma_2}\left((r-2)\,\mathscr{E}'^{2}_{\mathbf{h}_1}+(p-2)\,\mathscr{E}'^{2}_{\mathbf{h}_2}\right. \\
& \left.+(q-2)\,\mathscr{E}'^{2}_{\mathbf{h}_1+\mathbf{h}_2}\right)+\varrho_1\,, \qquad (6{\cdot}2)
\end{aligned}
$$

where

$$
\begin{aligned}
\varrho_1 = {} & -\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1}\left(\mathscr{E}'''_{h_1+h_2+k_2,\,h_2+k_1+k_2,\,\bar{h}_2+\bar{k}_2+l_1}\right. \\
& \qquad +\mathscr{E}'''_{h_1+h_2+l_2,\,\bar{h}_2+k_1+\bar{l}_2,\,h_2+l_1+l_2} \\
& \qquad \left.+\mathscr{E}_{h_1+\bar{k}_2+\bar{l}_2,\,k_1+k_2+l_2,\,k_2+l_1+l_2}\right) \\
& -\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_2}\left(\mathscr{E}'''_{h_1+h_2+k_1,\,h_1+k_1+k_2,\,\bar{h}_1+\bar{k}_1+l_2}\right. \\
& \qquad +\mathscr{E}'''_{h_1+h_2+l_1,\,\bar{h}_1+k_2+\bar{l}_1,\,h_1+l_1+l_2} \\
& \qquad \left.+\mathscr{E}'''_{h_2+\bar{k}_1+\bar{l}_1,\,k_1+k_2+l_1,\,k_1+l_1+l_2}\right) \\
& -\frac{\sigma_8^{1/2}}{\sigma_4}\,\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\left(\mathscr{E}'''_{h_1+\bar{k}_2,\,\bar{h}_2+k_1,\,h_2+k_2+l_1+l_2}\right. \\
& \qquad +\mathscr{E}'''_{h_1+\bar{l}_2,\,h_2+k_1+k_2+l_2,\,\bar{h}_2+l_1} \\
& \qquad \left.+\mathscr{E}'''_{h_1+h_2+k_2+l_2,\,k_1+\bar{l}_2,\,\bar{k}_2+l_1}\right)+\ldots\,. \qquad (6{\cdot}3)
\end{aligned}
$$

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

$$
\begin{aligned}
{}_6R'_{2,\,0} = {} & -\frac{\sigma_8^{1/2}}{\sigma_4}\left(\mathscr{E}'''_{h+k,\,h+k,\,\bar{h}+\bar{k}}+\mathscr{E}'''_{h+l,\,\bar{h}+\bar{l},\,h+l}+\mathscr{E}'''_{\bar{k}+\bar{l},\,k+l,\,k+l}\right) \\
& +\frac{4\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\,\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}-\frac{\sigma_4}{2C_1\sigma_2^2} \\
& \qquad \times(8C_1-6C_2+C_3)\,\mathscr{E}'^{2}_{\mathbf{h}} \\
& -\frac{4\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2)+\frac{\sigma_4}{16C_1^2\sigma_2^2} \\
& \qquad \times\left((2C_1-C_2)^2+4C_1(8C_1-6C_2+C_3)\right)+\ldots\,, \qquad (6{\cdot}4)
\end{aligned}
$$

and

$$
{}_6R'_{3,\,0} = \frac{\sigma_4^{1/2}}{8C_1\sigma_2}(2C_1-C_2)\left(\mathscr{E}'^{2}_{\mathbf{h}_1}+\mathscr{E}'^{2}_{\mathbf{h}_2}+\mathscr{E}'^{2}_{\mathbf{h}_1+\mathbf{h}_2}\right)+\varrho_1\,. \qquad (6{\cdot}5)
$$

For the space groups *Immm*, *Ibam*, *Imma* and *Ibca*, we have

$$R_{2,\,0} = {}_1R_{2,\,0}+{}_6R_{2,\,0}+\ldots\,, \qquad (6{\cdot}6)$$

$$R_{3,\,0} = {}_1R_{3,\,0}+{}_6R_{3,\,0}+\ldots\,, \qquad (6{\cdot}7)$$

$$R'_{2,\,0} = {}_1R'_{2,\,0}+{}_6R'_{2,\,0}+\ldots\,, \qquad (6{\cdot}8)$$

$$R'_{3,\,0} = {}_1R'_{3,\,0}+{}_6R'_{3,\,0}+\ldots\,, \qquad (6{\cdot}9)$$

where ${}_1R_{2,\,0}$, ${}_1R_{3,\,0}$, ${}_1R'_{2,\,0}$ 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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