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Structure Invariants and Seminvariants for Non-Centrosymmetric Space Groups

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The nature of the dependence of phase on the choice of origin is clarified for the non-centrosymmetric space groups by means of special linear combinations of the phases, the structure invariants and seminvariants. The theory yields simple answers to the following questions: Which phases have values determined uniquely by the crystal structure and independent of the choice of origin? If the values of certain phases are specified, what phases have values which are then uniquely determined by the structure? The values of which phases are to be specified in order to fix the origin uniquely?

Simple procedures for fixing the origin by suitably specifying the values of certain phases are described in detail.

1. Introduction

With the recent development of direct methods of phase determination the problem of choosing an origin by suitably specifying the values of an appropriate set of phases has assumed greater importance. The complete solution of this problem for the centrosymmetric space groups by means of the structure invariants and seminvariants has been given in our Monograph (Hauptman & Karle, 1953). This paper is devoted to the solution of the same problem for the non-centrosymmetric space groups. Owing to limitations of space, only a few typical proofs are given. However, the definitions and theorems are here arranged in logical order, and most of the missing proofs may be readily supplied.

A preliminary section showing the relation of this problem to the phase problem is given first.

2. The phase problem

The structure factor $F_{\mathbf{h}}$ is defined by means of

$$F_{\mathbf{h}} = |F_{\mathbf{h}}| \exp [i\varphi_{\mathbf{h}}] = X+iY \;, \qquad (2\cdot1)$$

$$X = \sum_{j=1}^{N/n} f_{j\mathbf{h}}\xi(\mathbf{h}, x_j, y_j, z_j) \;, \qquad (2\cdot2)$$

$$Y = \sum_{j=1}^{N/n} f_{j\mathbf{h}}\eta(\mathbf{h}, x_j, y_j, z_j) \;, \qquad (2\cdot3)$$

where N is the number of atoms in the unit cell, n is the order of the space group, $f_{j\mathbf{h}}$ is the atomic scattering factor, x_j, y_j, z_j are the coordinates of the jth atom, and ξ and η are trigonometric functions which depend upon the space group, e.g. for $P1$

$$\xi = \cos 2\pi(hx+ky+lz) \;, \qquad (2\cdot4)$$

$$\eta = \sin 2\pi(hx+ky+lz) \;. \qquad (2\cdot5)$$

Roughly speaking, the phase problem is the problem of determining the phases $\varphi_{\mathbf{h}}$ of the structure factors $F_{\mathbf{h}}$, defined by (2·1)–(2·3), given the magnitudes of the $F_{\mathbf{h}}$ and the values of the $f_{j\mathbf{h}}$ for a sufficiently large number of vectors $\mathbf{h}$.

The crystal structure alone does not, however, determine the values of all the phases (see, for example, Okaya & Nitta, 1952), because (2·1)–(2·3) imply that an appropriate origin has been selected. In fact, both the functional forms of ξ and η and the values of the atomic coordinates x_j, y_j, z_j depend upon the choice of origin. The magnitude $|F_{\mathbf{h}}|$ is, of course, independent of the choice of origin. However, as will be seen, there always exist certain linear combinations of the phases whose values (reduced modulo 2π, but always in the interval $-\pi < \varphi \leqslant \pi$) depend upon the structure alone and are independent of the choice of permissible origin (to be precisely defined later), and therefore of the functional form of the structure factor also. In analogy with centrosymmetric structures, we shall call these linear combinations of the phases the *structure invariants*. Furthermore, *for a fixed functional form of the structure factor* (i.e. for ξ and η), there always exist certain linear combinations of the phases whose values (again reduced modulo 2π) depend upon the structure alone and are independent of the choice of origin permitted by the chosen functional form for the structure factor. These linear combinations of the phases will be called the *structure seminvariants*. It will be seen that the structure seminvariants are independent of the chosen fixed functional form for the structure factor. While the structure seminvariants are determined by the space group and the choice of unit cell, their *values*, for a given structure, do depend on the chosen functional form for the structure factor. Evidently every structure invariant is also a structure seminvariant. In fact those structure seminvariants whose values are independent of the chosen functional form for the structure factor coincide with the structure invariants.

Although the crystal structure determines the values of the structure invariants, the magnitudes of the structure factors do not. In fact, if S is any structure then the enantiomorphous structure S', obtained by reflecting S through a point, has the same set of structure factor magnitudes as S.* However, as will be seen, the sign of any structure invariant for S is opposite to that of the corresponding invariant for S' (with the trivial exception that the value of a structure invariant is π for both structures). In other words the magnitudes of the structure factors determine only the magnitudes of the structure invariants. It is therefore desirable to introduce a new concept, that of the *intensity invariant*. The intensity invariants are those structure invariants whose values, *as a consequence of the space-group symmetry*, are either 0 or π. Hence any intensity invariant not only has a unique value independent of the choice of permissible origin but also of the choice of structure S or S'. In short, the values of the intensity invariants depend only on the magnitudes of the structure factors.

In formulating the phase problem it is not only necessary to take into account the need to specify the origin† but also to decide between the two enantiomorphous structures S and S'. In order to distinguish between the structures S and S' it is sufficient to specify arbitrarily the sign of any one structure invariant the magnitude of which is different from 0 and π (cf. chap. 6 of our Monograph).

The phase problem may be accurately described as the problem of determining the values of the structure invariants for either of the two enantiomorphous structures S, S' once a sufficiently large number of structure-factor magnitudes has been given (assuming as always that the atomic structure factors are known). Alternatively, the phase problem is the problem of determining the values of the structure seminvariants for either of the two enantiomorphous structures S, S', for each fixed functional form of structure factor, once a sufficiently large number of structure-factor magnitudes is known. The phases may then be obtained from the values of the structure seminvariants (or invariants) by fixing the origin. To show how this may be done by suitably specifying the values of an appropriate set of phases is a major aim of this paper.

3. Linear dependence and independence

First the concept of linear dependence modulo $\boldsymbol{\omega} = (\omega_1, \omega_2, \ldots, \omega_p)$, where the ω_i are arbitrary integers, is introduced since it permits the statement of general conclusions in a convenient and concise fashion. In the case that the ω_i are all zero this concept coincides with the ordinary one of linear dependence. If the ω_i are all equal to 2 this concept reduces to that of linear dependence modulo 2 previously described in chap. 2 of our Monograph. We shall need the more general concept in which the ω_i are arbitrary integers.

We discuss vectors $\mathbf{h} = (h_1, h_2, \ldots, h_p)$ all of whose p components are integers. The vector $\mathbf{h}$ is said to be divisible by $\boldsymbol{\omega}$ if the following two conditions are fulfilled:

1. $\omega_i = 0$ implies that $h_i = 0$;
2. $\omega_i \neq 0$ implies that h_i is divisible by ω_i.

In short $\mathbf{h}$ is divisible by $\boldsymbol{\omega}$ if there exist p integers q_i, $i = 1, 2, \ldots, p$, such that $h_i = q_i\omega_i$, $i = 1, 2, \ldots, p$. We then write

$$\mathbf{h} \equiv 0 \pmod{\boldsymbol{\omega}} \tag{3·1}$$

and say that $\mathbf{h}$ is congruent to zero modulo $\boldsymbol{\omega}$. In particular, taking $p = 1$, the integer h is congruent to zero modulo 0 if, and only if, $h = 0$; h is congruent to zero modulo $\omega \neq 0$ if, and only if, h is divisible by ω. If $\mathbf{h}$ is not congruent to zero modulo $\boldsymbol{\omega}$ then $\mathbf{h}$ is said to be incongruent to zero modulo $\boldsymbol{\omega}$. Two vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ are congruent modulo $\boldsymbol{\omega}$ if the difference $\mathbf{h}_1 - \mathbf{h}_2$ is divisible by $\boldsymbol{\omega}$; and the notation

$$\mathbf{h}_1 \equiv \mathbf{h}_2 \pmod{\boldsymbol{\omega}} \tag{3·2}$$

is used.

A set of n vectors $\mathbf{h}_j$, $j = 1, 2, \ldots, n$, $(n \geqslant 1)$, is said to be linearly dependent modulo $\boldsymbol{\omega}$ if there exists a set of n integers a_j, $j = 1, 2, \ldots, n$, at least one of which is incongruent to zero modulo ω_i for every $i (i = 1, 2, \ldots, p)$, such that

$$\sum_{j=1}^{n} a_j \mathbf{h}_j \equiv 0 \pmod{\boldsymbol{\omega}}\,. \tag{3·3}$$

Otherwise the set $\mathbf{h}_j$ is said to be linearly independent modulo $\boldsymbol{\omega}$.

The vector $\mathbf{h}$ is linearly dependent modulo $\boldsymbol{\omega}$ on, or linearly independent modulo $\boldsymbol{\omega}$ of, the set $\mathbf{h}_j$, $j = 1, 2, \ldots, n$ $(n \geqslant 1)$, according as there exist or there do not exist n integers a_j, $j = 1, 2, \ldots, n$, some or all of which may be zero, such that

$$\mathbf{h} \equiv \sum_{j=1}^{n} a_j \mathbf{h}_j \pmod{\boldsymbol{\omega}}\,. \tag{3·4}$$

In particular, any vector $\mathbf{h}$ divisible by $\boldsymbol{\omega}$ is linearly dependent modulo $\boldsymbol{\omega}$ on any set of vectors since every a_j in (3·4) may then be taken equal to zero.

In case $\omega_i = 0$ for every i our concepts reduce to ordinary linear dependence and independence, and the term 'modulo $\boldsymbol{\omega}$' will usually be omitted. The following two theorems are well known:

THEOREM 3·1. If $n > p$, the set of n vectors $\mathbf{h}_j$, $j = 1, 2, \ldots, n$, is linearly dependent.

THEOREM 3·2. If $n \leqslant p$, the set of n vectors $\mathbf{h}_j = (h_{j1}, h_{j2}, \ldots, h_{jp})$, $j = 1, 2, \ldots, n$, is linearly dependent if, and only if, every $n \times n$ sub-determinant of the $n \times p$ matrix

* We assume in this paper that the solution to the phase problem is essentially unique, i.e. that S and S' are the only structures having the given set of structure-factor magnitudes.

† We assume a fixed reference frame except for translations, and the problem of distinguishing between permissible reference frames (when they are distinct) is postponed (Hypothesis B, § 7, footnote).

$$H = \begin{pmatrix} h_{11} & h_{12} & \dots & h_{1p} \\ h_{21} & h_{22} & \dots & h_{2p} \\ \dots & \dots & \dots & \dots \\ h_{n1} & h_{n2} & \dots & h_{np} \end{pmatrix} \quad (3\cdot5)$$

vanishes.

4. Rational dependence and independence

The vector $\mathbf{h}$ is rationally dependent modulo $\boldsymbol{\omega}$ on, or rationally independent modulo $\boldsymbol{\omega}$ of, the set $\mathbf{h}_j, j = 1, 2, \dots, n, (n \geqslant 1)$, according as there exist or there do not exist n rational numbers $a_j, j=1,2,\dots,n$, some or all of which may be zero, such that

$$\mathbf{h} \equiv \sum_{j=1}^{n} a_j \mathbf{h}_j \pmod{\boldsymbol{\omega}} . \quad (4\cdot1)$$

The following theorem is an immediate consequence of the previous definitions.

THEOREM 4·1. If the vector $\mathbf{h}$ is linearly dependent modulo $\boldsymbol{\omega}$ on the set $\mathbf{h}_j, j = 1, 2, \dots, n, n \geqslant 1$, then $\mathbf{h}$ is rationally dependent modulo $\boldsymbol{\omega}$ on the set $\mathbf{h}_j$.

The converse of Theorem 4·1 is not true. However, we obtain a partial converse of this theorem by means of the important concept of the primitive set.

5. Primitive sets

Let the set M of n vectors $\mathbf{h}_j = (h_{j1}, h_{j2}, \dots, h_{jp})$, $j = 1, 2, \dots, n$, be given. If the set of vectors $\mathbf{h}_j$ is linearly dependent we define the modulus m of the set $\mathbf{h}_j$ to be zero. If the set $\mathbf{h}_j$ is linearly independent then, by Theorem 3·1, $n \leqslant p$, and the modulus m of the set $\mathbf{h}_j$ is defined to be the greatest common divisor of all $n \times n$ sub-determinants of the $n \times p$ matrix H, (3·5), not all of whose $n \times n$ sub-determinants vanish (Theorem 3·2). We shall call m also the modulus of the matrix H. If $m = 1$, then the set of n vectors $\mathbf{h}_j$ is said to be primitive. In case $m = 0$, whence the rank of the matrix H is $n' < n$, then the set M of n vectors $\mathbf{h}_j$ will also be called primitive provided that there exists a subset M' of M, consisting of n' vectors, which constitutes a primitive linearly independent basis for M, i.e. every vector of M is rationally dependent on the set of n' vectors M'. In particular, if $n = p$, then the linearly independent set $\mathbf{h}_j$ is primitive if, and only if, the determinant of H is ± 1.

The importance of the notion of primitive sets is due to the following fundamental theorem, a partial converse of Theorem 4·1 when every $\omega_i = 0$.

THEOREM 5·1. If the vector $\mathbf{h} = (h_1, h_2, \dots, h_p)$ is rationally dependent on the primitive, linearly independent set $\mathbf{h}_j, j = 1, 2, \dots, n, 1 \leqslant n \leqslant p$, then $\mathbf{h}$ is linearly dependent on the set $\mathbf{h}_j$.

Proof: Since $\mathbf{h}$ is rationally dependent on the set $\mathbf{h}_j$, there exist n rational numbers $a_j, j = 1, 2, \dots, n$, such that

$$\mathbf{h} = \sum_{j=1}^{n} a_j \mathbf{h}_j . \quad (5\cdot1)$$

Write $\mathbf{a} = (a_1, a_2, \dots, a_n)$. Then, using matrix notation, (5·1) becomes

$$\mathbf{h} = \mathbf{a}H , \quad (5\cdot2)$$

where H is given by (3·5) and the product $\mathbf{a}H$ means matrix multiplication. Since the linearly independent set $\mathbf{h}_j$ is primitive, the modulus of H is unity. Hence (Theorem H, Hauptman, 1954) there exists a $p \times n$ matrix Y with integer elements such that HY is the $n \times n$ identity matrix. Then (5·2) implies

$$\mathbf{h}Y = \mathbf{a}HY = \mathbf{a} . \quad (5\cdot3)$$

Since the elements of $\mathbf{h}$ and Y are integers, we conclude that the elements a_j of $\mathbf{a} = \mathbf{h}Y$ are also integers. In view of (5·1), $\mathbf{h}$ is linearly dependent on the set $\mathbf{h}_j$.

Next, let there be given a set of n vectors $\mathbf{h}_j$ and let at least one component of $\boldsymbol{\omega} = (\omega_1, \omega_2, \dots, \omega_p)$ be equal to zero. Suppress those components (if any) of each of the n vectors $\mathbf{h}_j$ the corresponding components of which in $\boldsymbol{\omega}$ are different from zero. We obtain the derived set of n vectors $\mathbf{h}'_j = (h'_{j1}, h'_{j2}, \dots, h'_{jp'})$, $j = 1, 2, \dots, n$, where $p' \geqslant 1$ is the number of those components in $\boldsymbol{\omega}$ which are equal to zero. The given set $\mathbf{h}_j$ is said to be primitive modulo $\boldsymbol{\omega}$ if the derived set $\mathbf{h}'_j$ is primitive. Evidently, if every $\omega_i = 0$, $i = 1, 2, \dots, p$, then the notion of primitive set modulo $\boldsymbol{\omega}$ reduces to that of primitive set.

Let the set of n vectors $\mathbf{h}_j, j = 1, 2, \dots, n$, be linearly independent, and let $n < p$. It is well known that there exists a vector $\mathbf{h}_{n+1}$ such that the set of $n+1$ vectors $\mathbf{h}_j, j = 1, 2, \dots, n+1$, is also linearly independent. We shall make important use of the following extension of this result.

THEOREM 5·2. There exists a primitive linearly independent set $\mathbf{h}$, consisting of a single vector. Let the linearly independent set of n vectors $\mathbf{h}_j, j=1, 2, \dots, n$, where $n < p$, be primitive. Then there exists a vector $\mathbf{h}_{n+1}$ such that the set of $n+1$ vectors $\mathbf{h}_j, j=1, 2, \dots, n+1$, is also primitive and linearly independent.

6. Equivalence

In general the functions ξ and η which define the structure factor F (equations (2·1)–(2·3)) for each space group depend upon the choice of origin. Two origins will be called equivalent if the functional forms for F to which they give rise are identical. In other words, two origins are equivalent if they are geometrically related in the same way to all the symmetry elements.

We retain as primary origin the one selected in *International Tables for X-ray Crystallography*, vol. 1, 1952. In each space group only certain points, related in a particularly simple way to the symmetry elements, can be chosen as possible origins if full advantage of the space-group symmetry is to be taken. For centrosymmetric space groups the permissible origins were defined to be the eight points

$$\varepsilon_1, \varepsilon_2, \varepsilon_3;\ \varepsilon_i = 0 \text{ or } \tfrac{1}{2},\ i = 1, 2, 3 , \quad (6\cdot1)$$

which, for primitive unit cells, coincide with the centers of symmetry. For non-centrosymmetric space groups the permissible origins are defined to be those points which are equivalent to at least one of the eight points (6·1). Only in this way do we make maximum use of the space-group symmetry. To allow other points as permissible origins would lead to fewer structure invariants, viz. those appropriate to space groups which are proper subgroups of the space group in question.

The concept of equivalent origins leads to the notion of *equivalence classes*. The set of all permissible origins may be grouped into classes, and any two origins in any class are equivalent while no origin in one class is equivalent to any origin in a different class.

As previously pointed out, the values of only the structure invariants are determined by the structure, while the values of the phases depend also on the choice of permissible origin. It will be seen later that the origin may be chosen by first selecting the functional form for the structure factor, i.e. an equivalence class, and then by specifying in a suitable manner the values of the phases of an appropriate set of structure factors.

7. The three categories of non-centrosymmetric space groups

Our discussion is restricted to primitive unit cells since we thereby avoid the unnecessary complexities resulting from the choice of non-primitive unit cells. In *International Tables for X-ray Crystallography*, vol. 1, 1952, the unit cell is chosen to be primitive for 94 of the 138 non-centrosymmetric space groups. However, for the remaining 44 space groups, structure factors appropriate to the choice of a primitive unit cell are readily obtained. Once this is done our methods become applicable to these space groups also. Alternatively, since the simple transformations from primitive unit cells to the conventional non-primitive unit cells are well known, our results are readily interpreted in terms of the latter choice of unit cell. In the monoclinic system we have chosen the second setting with b axis unique.

The structure factor for the general non-centrosymmetric crystal having N atoms per unit cell may be written.

$$F_{\mathbf{h}} = \sum_{j=1}^{N} f_{j\mathbf{h}} \exp\,[2\pi i(hx_j+ky_j+lz_j)]\,, \qquad (7\cdot1)$$

where the atomic structure factor $f_{j\mathbf{h}}$ is a function of $\mathbf{h}$, and the coordinates of the jth atom are x_j, y_j, z_j. If the origin is shifted to a different point having coordinates x_0, y_0, z_0 with respect to the first origin, then x_j, y_j, z_j in (7·1) are replaced by $x_j-x_0, y_j-y_0, z_j-z_0$. It is readily verified that $F_{\mathbf{h}}$ in (7·1) is then replaced by

$$F'_{\mathbf{h}} = F_{\mathbf{h}} \exp\,[-2\pi i(hx_0+ky_0+lz_0)]\,, \qquad (7\cdot2)$$

i.e. $F_{\mathbf{h}}$ is multiplied by $\exp\,[-2\pi i(hx_0+ky_0+lz_0)]$. In short, the magnitude of $F_{\mathbf{h}}$ remains unchanged while the phase $\varphi_{\mathbf{h}}$ of $F_{\mathbf{h}}$ is replaced by

$$\varphi'_{\mathbf{h}} = \varphi_{\mathbf{h}} - 2\pi(hx_0+ky_0+lz_0).$$

As with centrosymmetric space groups, the non-centrosymmetric space groups fall into three different categories depending upon the number of equivalence classes. Category 1 consists of those space groups having one equivalence class, Category 2 of those space groups having two equivalence classes, and Category 3 of those space groups having four equivalence classes. As shown in Table 1, each category is further subdivided into several types depending upon the nature of the equivalence classes. Each type is clearly characterized by row 6 of Table 1, the equivalence classes being defined by the boxes with solid lines.

We give next several definitions which are found to be convenient.

Definition 7·1. Two numbers a and b are said to be equivalent if the difference $a-b$ is an integer; the notation $a \equiv b$ is used. In particular a is an integer if, and only if, $a \equiv 0$.

Definition 7·2. To each type described in Table 1 we associate a vector $\boldsymbol{\omega}_i$ called the invariant modulus and a vector $\boldsymbol{\omega}_s$ called the seminvariant modulus and defined by rows 7 and 8 respectively of Table 1. For Category 1 the invariant modulus coincides with the seminvariant modulus and will be referred to simply as the modulus $\boldsymbol{\omega}$.

Definition 7·3. For each of the types described in Table 1, the vectors $\mathbf{h}_i$ and $\mathbf{h}_s$, associated invariantly and seminvariantly respectively with the phase $\varphi_{\mathbf{h}}$, are defined by rows 9 and 10 of Table 1. For Category 1, $\mathbf{h}_i = \mathbf{h}_s = \mathbf{h}$.

Definition 7·4. For each of the types described in Table 1, a set of phases is said to be linearly dependent or independent according as the set of invariantly associated vectors is linearly dependent or independent modulo $\boldsymbol{\omega}_i$, where $\boldsymbol{\omega}_i$ is the invariant modulus of the type. The phase $\varphi_{\mathbf{h}}$ is linearly (rationally) dependent on, or linearly (rationally) independent of, the set of phases $\varphi_{\mathbf{h}_j}$ according as the vector invariantly associated with $\varphi_{\mathbf{h}}$ is linearly (rationally) dependent modulo $\boldsymbol{\omega}_i$ on, or linearly (rationally) independent modulo $\boldsymbol{\omega}_i$ of, the set of vectors invariantly associated with the set $\varphi_{\mathbf{h}_j}$.

Definition 7·5. For each of the types described in Table 1, a set of phases $\varphi_{\mathbf{h}_j}$ is said to be linearly semi-dependent or semi-independent according as the set of seminvariantly associated vectors is linearly dependent or independent modulo $\boldsymbol{\omega}_s$, where $\boldsymbol{\omega}_s$ is the seminvariant modulus of the type. The phase $\varphi_{\mathbf{h}}$ is linearly (rationally) semi-dependent on, or linearly (rationally) semi-independent of, the set of phases $\varphi_{\mathbf{h}_j}$ according as the vector seminvariantly associated with $\varphi_{\mathbf{h}}$ is linearly (rationally) dependent modulo $\boldsymbol{\omega}_s$ on, or linearly (rationally) independent modulo $\boldsymbol{\omega}_s$ of, the set of vectors seminvariantly associated with the set $\varphi_{\mathbf{h}_j}$.

Table 1. *The permissible origins and equivalence classes for each of the thirteen types of non-centrosymmetric space groups*

A coordinate denoted by letter (x, y or z) takes on all values.

Category	1					2		3									
No. of equivalence classes	1					2		4									
Type	$1P000$	$1P202$	$1P020$	$1P222$	$1P220$	$2P20$	$2P22$	$3P30$	$3P32$		$3P_10$		$3P_12$		$3P_20$	$3P_22$	
Crystal system	Tri-clinic	Mono-clinic	Mono-clinic	Ortho-rhombic	Ortho-rhombic	Tetrag-onal	Tetrag-onal	Trig-onal	Trig-onal	Hexag-onal	Trig-onal	Hexag-onal	Trig-onal	Hexag-onal	Trig-onal	Trig-onal	Cubic
Space groups	$P1$	$P2$ $P2_1$	Pm Pc	$P222$ $P222_1$ $P2_12_12$ $P2_12_12_1$	$Pmm2$ $Pmc2_1$ $Pcc2$ $Pma2$ $Pca2_1$ $Pnc2$ $Pmn2_1$ $Pba2$ $Pna2_1$ $Pnn2$	$P4$ $P4_1$ $P4_2$ $P4_3$ $P4mm$ $P4bm$ $P4_2cm$ $P4_2nm$ $P4cc$ $P4nc$ $P4_2mc$ $P4_2bc$	$P\bar{4}$ $P422$ $P42_12$ $P4_122$ $P4_12_12$ $P4_222$ $P4_22_12$ $P4_322$ $P4_32_12$ $P\bar{4}2m$ $P\bar{4}2c$ $P\bar{4}2_1m$ $P\bar{4}2_1c$ $P\bar{4}m2$ $P\bar{4}c2$ $P\bar{4}b2$ $P\bar{4}n2$	$P3$ $P3_1$ $P3_2$ $P3m1$ $P3c1$	$P312$ $P3_112$ $P3_212$	$P\bar{6}$ $P\bar{6}m2$ $P\bar{6}c2$	$P31m$ $P31c$	$P6$ $P6_1$ $P6_5$ $P6_2$ $P6_4$ $P6_3$ $P6mm$ $P6cc$ $P6_3cm$ $P6_3mc$	$P321$ $P3_121$ $P3_221$	$P622$ $P6_122$ $P6_522$ $P6_222$ $P6_422$ $P6_322$ $P\bar{6}2m$ $P\bar{6}2c$	$R3$ $R3m$ $R3c$	$R32$	$P23$ $P2_13$ $P432$ $P4_232$ $P4_332$ $P4_132$ $P\bar{4}3m$ $P\bar{4}3n$
Permissible origins	x, y, z	$0, y, 0$ $0, y, \frac{1}{2}$ $\frac{1}{2}, y, 0$ $\frac{1}{2}, y, \frac{1}{2}$	$x, 0, z$ $x, \frac{1}{2}, z$	$0, 0, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $0, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$	$0, 0, 0$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$0, 0, z$ $\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z$ $\frac{1}{2}, 0, z$ $\frac{5}{6}, \frac{2}{3}, z$ $\frac{1}{6}, \frac{1}{3}, z$ $0, \frac{1}{2}, z$ $\frac{1}{3}, \frac{1}{6}, z$ $\frac{2}{3}, \frac{5}{6}, z$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{5}{6}, \frac{1}{6}, z$ $\frac{1}{6}, \frac{5}{6}, z$	$0, 0, 0$ $0, 0, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{5}{6}, \frac{2}{3}, 0$ $\frac{5}{6}, \frac{2}{3}, \frac{1}{2}$ $\frac{1}{6}, \frac{1}{3}, 0$ $\frac{1}{6}, \frac{1}{3}, \frac{1}{2}$	$0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{3}, \frac{1}{6}, 0$ $\frac{1}{3}, \frac{1}{6}, \frac{1}{2}$ $\frac{2}{3}, \frac{5}{6}, 0$ $\frac{2}{3}, \frac{5}{6}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{5}{6}, \frac{1}{6}, 0$ $\frac{5}{6}, \frac{1}{6}, \frac{1}{2}$ $\frac{1}{6}, \frac{5}{6}, 0$ $\frac{1}{6}, \frac{5}{6}, \frac{1}{2}$	$0, 0, z$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, z$		$0, 0, 0$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		x, x, x $x+\frac{1}{2}, x, x$ $x, x+\frac{1}{2}, x$ $x, x, x+\frac{1}{2}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	
Invariant modulus $\boldsymbol{\omega}_i$	(0, 0, 0)	(2, 0, 2)	(0, 2, 0)	(2, 2, 2)	(2, 2, 0)	(2, 2, 0)	(2, 2, 2)	(6, 6, 0)	(6, 6, 2)		(2, 2, 0)		(2, 2, 2)		(2, 2, 2, 0)	(2, 2, 2)	
Seminvariant modulus $\boldsymbol{\omega}_s$	(0, 0, 0)	(2, 0, 2)	(0, 2, 0)	(2, 2, 2)	(2, 2, 0)	(2, 0)	(2, 2)	(3, 0)	(3, 2)		(0)		(2)		(0)	(2)	
Vector $\mathbf{h}_i$ invariantly associated with $\varphi_{\mathbf{h}}$ or with $\mathbf{h} = (h, k, l)$	(h, k, l)					(h, k, l)		$(h+2k, 2h+k, l)$			(h, k, l)				$(h, k, l, h+k+l)$	(h, k, l)	
Vector $\mathbf{h}_s$ seminvariantly associated with $\varphi_{\mathbf{h}}$ or with $\mathbf{h} = (h, k, l)$	(h, k, l)					$(h+k, l)$		$(h-k, l)$			(l)				$(h+k+l)$		
For fixed form for structure factor, number of phases linearly semi-independent to be specified	3					2		2			1						

DEFINITION 7·6. For each of the types described in Table 1, a set of phases $\varphi_{\mathbf{h}_j}$ is said to be primitive if the set of invariantly associated vectors is primitive modulo ω_i, where ω_i is the invariant modulus of the type.

DEFINITION 7·7. For each of the types described in Table 1, a set of phases $\varphi_{\mathbf{h}_j}$ is said to be semi-primitive if the set of seminvariantly associated vectors is primitive modulo ω_s, where ω_s is the seminvariant modulus of the type.

Table 1 shows that the concepts of invariance and seminvariance coincide for Category 1.

It is now possible to state the following five fundamental theorems which summarize briefly some of the main results of this paper:

MAIN THEOREM 7·1. The crystal structure determines the values of all the structure invariants. For each fixed functional form for the structure factor, the crystal structure determines the values of all the structure seminvariants.

MAIN THEOREM 7·2. The value of any structure invariant for the structure S is the negative of the corresponding structure invariant for the enantiomorphous structure S' obtained by reflecting S through a point (with the trivial exception that a structure invariant may have the value π for both structures).

MAIN THEOREM 7·3. A sufficient number of structure factor magnitudes determines the magnitudes of all the structure invariants and the values of all the intensity invariants. The sign of any structure invariant, the value of which is different from 0 and π, may be specified arbitrarily. Once this is done (thus distinguishing between the two enantiomorphous structures S and S' permitted by the structure factor magnitudes) then the values (not merely the magnitudes) of all remaining structure invariants are uniquely determined by the structure-factor magnitudes. In addition, if a functional form for the structure factor is chosen, then the values of all the structure seminvariants are also uniquely determined.*

MAIN THEOREM 7·4. For each type the structure invariants are the linear combinations

$$\dot{\sum_{\mathbf{h}}} A_{\mathbf{h}}\varphi_{\mathbf{h}}\,, \tag{7·3}$$

where the $A_{\mathbf{h}}$ are integers satisfying

$$\sum_{\mathbf{h}} A_{\mathbf{h}}\mathbf{h}_i \equiv 0 \ (\mathrm{mod}\ \omega_i)\,, \tag{7·4}$$

$\mathbf{h}_i$ is the vector invariantly associated with the phase $\varphi_{\mathbf{h}}$, ω_i is the invariant modulus of the type, and the symbol $\dot{\sum}$ in (7·3) means (as always) that the sum in (7·3) is to be reduced modulo 2π and $-\pi < \dot{\sum\limits_{\mathbf{h}}} \leqslant \pi$.

* Main theorems 7·2 and 7·3 are valid also for the structure seminvariants provided that the functional form for the structure factor is fixed; hence provided that the space group does not belong to one of the 11 enantiomorphous pairs.

MAIN THEOREM 7·5. For each type the structure seminvariants are the linear combinations

$$\dot{\sum_{\mathbf{h}}} A_{\mathbf{h}}\varphi_{\mathbf{h}}\,, \tag{7·5}$$

where the $A_{\mathbf{h}}$ are integers satisfying

$$\sum_{\mathbf{h}} A_{\mathbf{h}}\mathbf{h}_s \equiv 0 \ (\mathrm{mod}\ \omega_s)\,, \tag{7·6}$$

$\mathbf{h}_s$ is the vector seminvariantly associated with the phase $\varphi_{\mathbf{h}}$, and ω_s is the seminvariant modulus of the type.

The remainder of this paper is devoted to spelling out in detail simple methods for selecting the origin for each of the thirteen types of non-centrosymmetric space groups. For each type in Categories 2 and 3 we give two procedures, first by means of the structure invariants and secondly by means of the structure seminvariants. Although, for some of the types, our methods are capable of yielding somewhat more general results than those we describe, we give, for the sake of brevity and clarity, only the simplest procedures.

All the remaining theorems of this paper are valid under either one of the following hypotheses:

Hypothesis A: The crystal structure is given; or

Hypothesis B: A sufficiently large number of structure-factor magnitudes is given (so that, by Theorem 7·3, the magnitudes of all the structure invariants are determined) and the sign of any one structure invariant, the magnitude of which is different from 0 and π, has been arbitrarily specified (in accordance with Theorem 7·3).*

The role played by the primitive sets in leading to a unique choice of origin is especially noteworthy and should be emphasized at the start. If the set of phases whose values are specified is not primitive, then the values of certain of the remaining phases will not be uniquely determined.

8. The thirteen types of non-centrosymmetric space groups

8·01. *Type* 1*P*000

THEOREM 8·01·1. No single phase (except the trivial φ_{000}) is a structure invariant.

Proof: Theorem 7·4.

THEOREM 8·01·2. The value of any phase $\varphi_{\mathbf{h}_1}$, which is linearly independent, may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$

* In this way we distinguish the two enantiomorphous structures S, S' (when they are distinct), or the permissible reference frames (when they are distinct), or both. In the case that the magnitude of no structure invariant is different from 0 or π then their values are independent of the choice of enantiomorphous structure and of permissible reference frame. Thus the need of specifying the sign of a structure invariant does not arise in this case. The same remarks apply to the structure seminvariants provided that the functional form for the structure factor has been fixed.

which is linearly dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on $\varphi_{\mathbf{h}_1}$ is also linearly dependent on $\varphi_{\mathbf{h}_1}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_1}$, is primitive, i.e. provided that the greatest common divisor of h_1, k_1, and l_1 is unity.

Proof: This is a consequence of Theorems 7·2 and 7·4 since (7·2) implies

$$h_1x_0+k_1y_0+l_1z_0 \equiv \frac{1}{2\pi}(\varphi_{\mathbf{h}_1}-\varphi'_{\mathbf{h}_1}) , \qquad (8{\cdot}1)$$

an equation which has solutions x_0, y_0, z_0 (of necessity equivalent to 0, 0, 0) for arbitrary choice of value for $\varphi'_{\mathbf{h}_1}$, in view of the hypothesis that $\varphi_{\mathbf{h}_1}$ is linearly independent.

Theorem 8·01·3. The values of any two phases $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, constituting a linearly independent set, may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is also linearly dependent on this pair, whence its value is uniquely determined, provided that the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is primitive, i.e. provided that the greatest common divisor of

$$\begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix}, \quad \begin{vmatrix} h_1 & l_1 \\ h_2 & l_2 \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} k_1 & l_1 \\ k_2 & l_2 \end{vmatrix}$$

is unity.

Theorem 8·01·4. The values of any three phases $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, $\varphi_{\mathbf{h}_3}$, constituting a linearly independent set, may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the triple $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, $\varphi_{\mathbf{h}_3}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$, of necessity rationally dependent on the triple $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, $\varphi_{\mathbf{h}_3}$, is also linearly dependent on this triple, whence its value is uniquely determined, provided that the triple $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, $\varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that

$$\begin{vmatrix} h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 \\ h_3 & k_3 & l_3 \end{vmatrix} = \pm 1 .$$

8·02. *Type* 1*P*222

Theorem 8·02·1. A single phase $\varphi_{\mathbf{h}}$ is a structure invariant, i.e. its value is uniquely determined, if, and only if, h, k and l are all even.

Proof: Theorem 7·4.

Theorem 8·02·2. Any phase $\varphi_{\mathbf{h}_1}$, which is linearly independent, has just two possible values, and these differ from each other by π. Either one of these two values may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Proof: Equation (7·2) implies (8·1) where now the permissible origins x_0, y_0, z_0 coincide with the eight points (6·1). Hence any two different values for $\varphi'_{\mathbf{h}_1}$ differ by π, and either one of these two possible values may be realized by suitably choosing the origin since $\varphi_{\mathbf{h}_1}$ is linearly independent. The theorem then follows from Theorems 7·2 and 7·4.

Theorem 8·02·3. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases constituting a linearly independent set. In accordance with Theorem 8·02·2 either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen, and either one of the two possible values of $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is uniquely determined.

Theorem 8·02·4. Let $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, and $\varphi_{\mathbf{h}_3}$ be any three phases constituting a linearly independent set. In accordance with Theorem 8·02·2 either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen, either one of the two possible values of $\varphi_{\mathbf{h}_2}$ may be chosen, and either one of the two possible values of $\varphi_{\mathbf{h}_3}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly dependent on the triple $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, $\varphi_{\mathbf{h}_3}$, is uniquely determined.

8·03. *Type* 1*P*202

Theorem 8·03·1. A single phase $\varphi_{\mathbf{h}}$ is a structure invariant, i.e. its value is uniquely determined, if, and only if, h and l are both even and $k = 0$.

Proof: Theorem 7·4.

Theorem 8·03·2. Any phase $\varphi_{h_10l_1}$ which is linearly independent (i.e. h_1 and l_1 are not both even) has just two possible values, and these differ from each other by π. Either one of these two values may be chosen. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Theorem 8·03·3. Let h_3 and l_3 both be even. Then the value of any phase $\varphi_{\mathbf{h}_3}$ which is linearly independent (i.e. $k_3 \neq 0$) may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_3}$ (i.e. h and l are both even and k is divisible by k_3) is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on $\varphi_{\mathbf{h}_3}$ is also linearly dependent on $\varphi_{\mathbf{h}_3}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $k_3 = \pm 1$.

Theorem 8·03·4. Let $\varphi_{h_10l_1}$ and $\varphi_{h_20l_2}$ be any two phases constituting a linearly independent set. In accordance with Theorem 8·03·2 either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen, and either one of the two possible values of $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is uniquely determined.

Theorem 8·03·5. Let $k_1 = 0$ and h_3 and l_3 be both even. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ be any two phases constituting a linearly independent set (i.e. h_1 and l_1 are not both even, and $k_3 \neq 0$). In accordance with Theorems 8·03·2 and 8·03·3 either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen while the value of $\varphi_{\mathbf{h}_3}$ may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair

$\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is also linearly dependent on this pair, whence its value is uniquely determined, provided that the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $k_3 = \pm 1$.

THEOREM 8·03·6. Let $k_1 = k_2 = 0$ and h_3 and l_3 be both even. Let $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ and $\varphi_{\mathbf{h}_3}$ be any three phases constituting a linearly independent set. In accordance with Theorems 8·03·3 and 8·03·4 either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen and either one of the two possible values of $\varphi_{\mathbf{h}_2}$ may be chosen, while the value of $\varphi_{\mathbf{h}_3}$ may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the set $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ (i.e. k is a multiple of k_3) is uniquely determined. In view of Theorem 5·1 any phase $\varphi_{\mathbf{h}}$, of necessity rationally dependent on the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$, is also linearly dependent on this triple, whence its value is uniquely determined, provided that the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $k_3 = \pm 1$.

8·04. *Type* 1*P*020

THEOREM 8·04·1. A single phase $\varphi_{\mathbf{h}}$ is a structure invariant if, and only if, $h = l = 0$ and k is even.

Proof: Theorem 7·4.

THEOREM 8·04·2. Any phase φ_{0k_10}, which is linearly independent (i.e. k_1 is odd), has just two possible values, and these differ from each other by π. Either one of these two values may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_1}$ (i.e. $h = l = 0$ and k is odd) is uniquely determined.

THEOREM 8·04·3. Let k_2 be even. Then the value of any phase $\varphi_{\mathbf{h}_2}$ which is linearly independent (i.e. h_2 and l_2 are not both zero) may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_2}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on $\varphi_{\mathbf{h}_2}$ is also linearly dependent on $\varphi_{\mathbf{h}_2}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_2}$ is primitive, i.e. provided that h_2 and l_2 are relatively prime.

THEOREM 8·04·4. Let k_2 and k_3 be even. Then the values of any two phases $\varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$, constituting a linearly independent set, may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on the pair $\varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is also linearly dependent on this pair, whence its value is uniquely determined, provided that the pair is primitive, i.e. provided that

$$\begin{vmatrix} h_2 & l_2 \\ h_3 & l_3 \end{vmatrix} = \pm 1 .$$

THEOREM 8·04·5. Let $h_1 = l_1 = 0$ and k_2 be even. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases which constitute a linearly independent set (i.e. k_1 is odd and h_2 and l_2 are not both zero). In accordance with Theorems 8·04·2 and 8·04·3, either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen while the value of $\varphi_{\mathbf{h}_2}$ may be specified arbitrarily. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is also linearly dependent on this pair, whence its value is uniquely determined, provided that the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is primitive, i.e. provided that h_2 and l_2 are relatively prime.

THEOREM 8·04·6. Let $h_1 = l_1 = 0$ and k_2 and k_3 both be even. Let the three phases $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ constitute a linearly independent set, i.e. k_1 is odd and

$$\begin{vmatrix} h_2 & l_2 \\ h_3 & l_3 \end{vmatrix} \neq 0 .$$

In accordance with Theorems 8·04·4 and 8·04·6, either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen, while the values of $\varphi_{\mathbf{h}_2}$ and $\varphi_{\mathbf{h}_3}$ may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the set $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is uniquely determined. In view of Theorem 5·1 any phase $\varphi_{\mathbf{h}}$, of necessity rationally dependent on the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$, is also linearly dependent on this triple, whence its value is uniquely determined, provided that the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that

$$\begin{vmatrix} h_2 & l_2 \\ h_3 & l_3 \end{vmatrix} = \pm 1 .$$

8·05. *Type* 1*P*220

Evidently Theorems 8·03·1–8·03·6 for Type 1*P*202 are valid also for Type 1*P*220, except for the obvious changes involving the interchange of the second and third indices.

8·06. *Type* 2*P*20

The permissible origins coincide with those for Type 1*P*220. Hence Theorems 8·03·1–8·03·6 for Type 1*P*202 are valid also for Type 2*P*20, except for the changes involving the interchange of the second and third indices.

THEOREM 8·06·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant, i.e. for a fixed functional form for the structure factor its value is uniquely determined, if and only if $h+k$ is even and $l = 0$.

Proof: Theorem 7·5.

THEOREM 8·06·2. Let the functional form for the structure factor be fixed. Let $l_1 = 0$. Then any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. h_1+k_1 is odd) has just two possible values, and these differ from each other by π. Either one of these two values may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ (i.e. $l = 0$) is uniquely determined.

THEOREM 8·06·3. Let the functional form for the structure factor be fixed. Let h_2+k_2 be even. Then the value of any phase $\varphi_{\mathbf{h}_2}$ which is linearly semi-independent (i.e. $l_2 \neq 0$) may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_2}$ (i.e. $h+k$ is even and l is divisible by l_2) is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally semi-dependent on $\varphi_{\mathbf{h}_2}$ is also linearly semi-dependent on $\varphi_{\mathbf{h}_2}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_2}$ is semi-primitive, i.e. provided that $l_2 = \pm 1$.

Theorem 8·06·4. Let the functional form for the structure factor be fixed. Let $l_1 = 0$ and h_2+k_2 be even. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases which constitute a linearly semi-independent set (i.e. h_1+k_1 is odd and $l_2 \neq 0$). In accordance with Theorems 8·06·2 and 8·06·3, either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen while the value of $\varphi_{\mathbf{h}_2}$ may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$, of necessity rationally semi-dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, is also linearly semi-dependent on this pair, whence its value is uniquely determined, provided that the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is semi-primitive, i.e. provided that $l_2 = \pm 1$.

8·07. *Type* 2*P*22

The permissible origins coincide with those for Type 1*P*222. Hence Theorems 8·02·1–8·02·4 for Type 1*P*222 are valid also for Type 2*P*22.

Theorem 8·07·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, $h+k$ and l are both even.

Proof: Theorem 7·5.

Theorem 8·07·2. Let the functional form for the structure factor be fixed. Any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. h_1+k_1 and l_1 are not both even) has just two possible values; these differ from each other by π. Either one of these two values may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Theorem 8·07·3. Let the functional form for the structure factor be fixed. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases which constitute a linearly semi-independent pair. In accordance with Theorem 8·07·2, either one of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen, and either one of the two possible values of $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, is uniquely determined.

8·08. *Type* 3*P*30

Theorem 8·08·1. A single phase $\varphi_{\mathbf{h}}$ is a structure invariant if, and only if, $h \equiv k \equiv 0$ or 2 or 4 (mod 6) and $l = 0$.

Proof: Theorem 7·4.

Theorem 8·08·2. Let $l_1 = 0$ and $\varphi_{\mathbf{h}_1}$ be any phase which is linearly independent. Then $\varphi_{\mathbf{h}_1}$ has just six possible values, and these form an arithmetic progression with common difference equal to $\pi/3$. Any one of these six values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Theorem 8·08·3. Let $l_1 = l_2 = 0$ and let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases each of which is linearly independent and neither of which is linearly dependent on the other. (We note however that the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ is of necessity linearly dependent.) In accordance with Theorem 8·08·2, the value of $\varphi_{\mathbf{h}_1}$ may be arbitrarily chosen from a certain set of six numbers in arithmetic progression with common difference $\pi/3$. Once this is done then there remain only two possible values for $\varphi_{\mathbf{h}_2}$, and these differ from each other by π. Either one of these two possible values for $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ (i.e. $l = 0$) is uniquely determined.

Theorem 8·08·4. Let $h_3+2k_3 \equiv 2h_3+k_3 \equiv 0$ (mod 6) and let $\varphi_{\mathbf{h}_3}$ be any phase which is linearly independent (i.e. $l_3 \neq 0$). Then the value of $\varphi_{\mathbf{h}_3}$ may be arbitrarily specified. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_3}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on $\varphi_{\mathbf{h}_3}$ is also linearly dependent on $\varphi_{\mathbf{h}_3}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $l_3 = \pm 1$.

Theorem 8·08·5. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ be as in Theorems 8·08·2 and 8·08·4. Then the conclusions of Theorems 8·08·2 and 8·08·4 are valid. In addition, once the values of $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ have been specified in accordance with Theorems 8·08·2 and 8·08·4 then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_3}$ is uniquely determined.

Theorem 8·08·6. Let the phases $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$, and $\varphi_{\mathbf{h}_3}$ be as in Theorems 8·08·3 and 8·08·4. Then the conclusions of Theorems 8·08·3 and 8·08·4 hold. In addition, once the values of $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_2}$ and $\varphi_{\mathbf{h}_3}$ have been specified in accordance with Theorems 8·08·3 and 8·08·4, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is uniquely determined. Any phase $\varphi_{\mathbf{h}}$, of necessity rationally dependent on the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is also linearly dependent on this triple, whence its value is uniquely determined, provided that the triple is primitive, i.e. provided that $l_3 = \pm 1$.

Theorem 8·08·7. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, $h \equiv k$ (mod 3) and $l = 0$.

Proof: Theorem 7·5.

Theorem 8·08·8. Let the functional form for the structure factor be fixed. Let $l_1 = 0$. Any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. $h_1 \not\equiv k_1$ (mod 3)) has just three possible values, and these form an arithmetic progression with common difference equal to $2\pi/3$. Any one of these three values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ (i.e. $l=0$) is uniquely determined.

THEOREM 8·08·9. Let the functional form for the structure factor be fixed. Let $h_2 \equiv k_2 \pmod 3$ and let $\varphi_{\mathbf{h}_2}$ be any phase which is linearly semi-independent (i.e. $l_2 \neq 0$). Then the value of $\varphi_{\mathbf{h}_2}$ may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_2}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally semi-dependent on $\varphi_{\mathbf{h}_2}$ is also linearly semi-dependent on $\varphi_{\mathbf{h}_2}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_2}$ is semi-primitive, i.e. provided that $l_2 = \pm 1$.

THEOREM 8·08·10. Let the functional form for the structure factor be fixed. Let the phases $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ be as in Theorems 8·08·7 and 8·08·8 whence they constitute a linearly semi-independent pair. In accordance with Theorems 8·08·7 and 8·08·8, the value of $\varphi_{\mathbf{h}_1}$ may be chosen arbitrarily from a certain set of three numbers in arithmetic progression while the value of $\varphi_{\mathbf{h}_2}$ may be specified arbitrarily. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$, of necessity rationally semi-dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is also linearly semi-dependent on this pair, whence its value is uniquely determined, provided that the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is semi-primitive, i.e. provided that $l_2 = \pm 1$.

8·09. *Type* 3*P*32

THEOREM 8·09·1. A single phase $\varphi_{\mathbf{h}}$ is a structure invariant if, and only if, $h \equiv k \equiv 0$ or 2 or 4 (mod 6) and $l \equiv 0 \pmod 2$.

Proof: Theorem 7·4.

THEOREM 8·09·2. Let $l_1 \equiv 0 \pmod 2$ and $\varphi_{\mathbf{h}_1}$ be any phase which is linearly independent. Then $\varphi_{\mathbf{h}_1}$ has just six possible values, and these form an arithmetic progression with common difference equal to $\pi/3$. Any one of these six values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

THEOREM 8·09·3. Let $l_1 \equiv l_2 \equiv 0 \pmod 2$ and let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases each of which is linearly independent and neither of which is linearly dependent on the other. (As in Theorem 8·08·3 the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is of necessity linearly dependent.) In accordance with Theorem 8·09·2, the value of $\varphi_{\mathbf{h}_1}$ may be arbitrarily chosen from a certain set of six numbers in arithmetic progression with common difference $\pi/3$. Once this is done then there remain only two possible values for $\varphi_{\mathbf{h}_2}$, and these differ from each other by π. Either one of these two possible values for $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ (i.e. l is even) is uniquely determined.

THEOREM 8·09·4. Let $h_3+2k_3 \equiv 2h_3+k_3 \equiv 0 \pmod 6$ and let $\varphi_{\mathbf{h}_3}$ be any phase which is linearly independent (i.e. l_3 is odd). Then $\varphi_{\mathbf{h}_3}$ has just two possible values, and these differ from each other by π. Either one of these two values for $\varphi_{\mathbf{h}_3}$ may be chosen. Once this is done then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_3}$ is uniquely determined.

THEOREM 8·09·5. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ be as in Theorems 8·09·2 and 8·09·4. Then the conclusions of Theorems 8·09·2 and 8·09·4 are valid. In addition, once the values of $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ have been specified in accordance with Theorems 8·09·2 and 8·09·4 then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is uniquely determined.

THEOREM 8·09·6. Let the phases $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$, and $\varphi_{\mathbf{h}_3}$ be as in Theorems 8·09·3 and 8·09·4. Then the conclusions of Theorems 8·09·3 and 8·09·4 hold. In addition, once the values of $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$, and $\varphi_{\mathbf{h}_3}$ have been specified in accordance with Theorems 8·09·3 and 8·09·4, then the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly dependent on the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$, is uniquely determined.

THEOREM 8·09·7. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, $h \equiv k \pmod 3$ and $l \equiv 0 \pmod 2$.

Proof: Theorem 7·5.

THEOREM 8·09·8. Let the functional form for the structure factor be fixed. Let l_1 be even. Any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. $h_1 \not\equiv k_1 \pmod 3$) has just three possible values, and these form an arithmetic progression with common difference equal to $2\pi/3$. Any one of these three values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ (i.e. l is even) is uniquely determined.

THEOREM 8·09·9. Let the functional form for the structure factor be fixed. Let $h_2 \equiv k_2 \pmod 3$ and let $\varphi_{\mathbf{h}_2}$ be any phase which is linearly semi-independent (i.e. l_2 is odd). Then $\varphi_{\mathbf{h}_2}$ has just two possible values, and these differ from each other by π. Either one of these two values for $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done, then the value of any phase which is linearly semi-dependent on $\varphi_{\mathbf{h}_2}$ is uniquely determined.

THEOREM 8·09·10. Let the functional form for the structure factor be fixed. Let the phases $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ be as in Theorems 8·09·8 and 8·09·9 whence they constitute a linearly semi-independent pair. In accordance with Theorems 8·09·8 and 8·09·9, the value of $\varphi_{\mathbf{h}_1}$ may be chosen arbitrarily from a certain set of three numbers in arithmetic progression while the value of $\varphi_{\mathbf{h}_2}$ may be chosen arbitrarily from a certain set of two numbers. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$, is uniquely determined.

8·10. *Type* $3P_10$

For Type $3P_10$ the permissible origins coincide with those for Type 1*P*220. Hence Theorems 8·03·1–8·03·6 for Type 1*P*202 are valid also for Type $3P_10$, except for the changes involving the interchange of the second and third indices.

THEOREM 8·10·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, $l = 0$.

THEOREM 8·10·2. Let the functional form for the structure factor be fixed. The value of any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. $l_1 \neq 0$) may be specified arbitrarily. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$, of necessity rationally semi-dependent on $\varphi_{\mathbf{h}_1}$, is also linearly semi-dependent on $\varphi_{\mathbf{h}_1}$, whence its value is uniquely determined, provided that the phase $\varphi_{\mathbf{h}_1}$ is semi-primitive, i.e. provided that $l_1 = \pm 1$.

8·11. *Type* $3P_12$

For Type $3P_12$ the permissible origins coincide with those for Type $1P222$. Hence Theorems 8·02·1–8·02·4 for Type $1P222$ are valid also for Type $3P_12$.

Theorem 8·11·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, l is even.

Theorem 8·11·2. Let the functional form for the structure factor be fixed. Any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. l_1 is odd) has just two possible values, and these differ from each other by π. Either one of these two values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_1}$, is uniquely determined.

8·12. *Type* $3P_20$

Theorem 8·12·1. A single phase $\varphi_{\mathbf{h}}$ is a structure invariant if, and only if, $h \equiv k \equiv l \equiv 0 \pmod 2$ and $h+k+l = 0$.

Proof: Theorem 7·4.

Theorem 8·12·2. Let $h_1+k_1+l_1 = 0$, and let $\varphi_{\mathbf{h}_1}$ be any phase which is linearly independent. Then $\varphi_{\mathbf{h}_1}$ has just two possible values, and these differ from each other by π. Either one of these two values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Theorem 8·12·3. Let $h_1+k_1+l_1 = h_2+k_2+l_2 = 0$ and let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ be any two phases which constitute a linearly independent pair. In accordance with Theorem 8·12·2 either one of the two possible values for $\varphi_{\mathbf{h}_1}$ may be chosen, and either one of the two possible values for $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done, then the value of any phase which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ is uniquely determined.

Theorem 8·12·4. Let $h_3+k_3+l_3$ be odd, whence the phase $\varphi_{\mathbf{h}_3}$ is linearly independent. Then the value of $\varphi_{\mathbf{h}_3}$ may be specified arbitrarily. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on $\varphi_{\mathbf{h}_3}$ is uniquely determined. In view of Theorem 5·1, any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on $\varphi_{\mathbf{h}_3}$ is also linearly dependent on $\varphi_{\mathbf{h}_3}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $h_3+k_3+l_3 = \pm 1$.

Theorem 8·12·5. Let $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ be as in Theorems 8·12·2 and 8·12·4. Then the conclusions of Theorems 8·12·2 and 8·12·4 are valid. In addition, once the values of $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_3}$ have been specified in accordance with Theorems 8·12·2 and 8·12·4, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is uniquely determined. Any phase $\varphi_{\mathbf{h}}$ which is rationally dependent on the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is also linearly dependent on this pair, whence its value is uniquely determined, provided that the pair $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $h_3+k_3+l_3 = \pm 1$.

Theorem 8·12·6. Let the three phases $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$, and $\varphi_{\mathbf{h}_3}$ be as in Theorems 8·12·2–8·12·4. Then the conclusions of Theorems 8·12·2–8·12·4 are valid. In addition, once the values of $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$ and $\varphi_{\mathbf{h}_3}$ have been specified in accordance with Theorems 8·12·2–8·12·4, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly dependent on the set $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is uniquely determined. Any phase $\varphi_{\mathbf{h}}$, of necessity rationally dependent on the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$, is also linearly dependent on this triple, whence its value is uniquely determined, provided that the triple $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}, \varphi_{\mathbf{h}_3}$ is primitive, i.e. provided that $h_3+k_3+l_3 = \pm 1$.

Theorem 8·12·7. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, $h+k+l = 0$.

Proof: Theorem 7·5.

Theorem 8·12·8. Let the functional form for the structure factor be fixed. The value of any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. $h_1+k_1+l_1 \neq 0$) may be specified arbitrarily. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined. Any phase $\varphi_{\mathbf{h}}$, of necessity rationally semi-dependent on $\varphi_{\mathbf{h}_1}$, is also linearly semi-dependent on $\varphi_{\mathbf{h}_1}$, whence its value is uniquely determined, provided that $\varphi_{\mathbf{h}_1}$ is semi-primitive, i.e. provided that $h_1+k_1+l_1 = \pm 1$.

8·13. *Type* $3P_22$

For Type $3P_22$ the permissible origins coincide with those for Type $1P222$. Hence Theorems 8·02·1–8·02·4 for Type $1P222$ are valid also for Type $3P_22$.

Theorem 8·13·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant if, and only if, $h+k+l$ is even.

Theorem 8·13·2. Let the functional form for the structure factor be fixed. Any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. $h_1+k_1+l_1$ is odd) has just two possible values, and these differ from each other by π. Either one of these two values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done, then the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_1}$, is uniquely determined.

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