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Seminvariants for Non-centrosymmetric Space Groups with Conventional Centered Cells

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The relationship of phase to the choice of origin, enantiomorph or frame of reference is clarified for those non-centrosymmetric space groups for which the conventional unit cell is not primitive. The theory employs special linear combinations of the phases, the structure seminvariants. Simple procedures are developed for selecting the origin by first fixing the functional form of the structure factor, then specifying the sign of a seminvariant when required, and, finally, specifying arbitrarily the values of a suitable set of phases.

This paper completes the study of the seminvariants for all the space groups.

1. Introduction

In the direct determination of phases from the observed intensities it is necessary to relate the values of the phases to the choice of origin, reference frame and enantiomorph. This problem has already been treated for the centrosymmetric space groups (Hauptman & Karle, 1953, 1959) and for the non-centrosymmetric space groups for which the conventional unit cell is primitive (Hauptman & Karle, 1956). It was found that certain linear combinations of the phases, the structure seminvariants, play a fundamental role in these studies. The seminvariants show which linear combinations are determined by the intensities alone and how specifications of phases are to be made to fix the origin, frame and enantiomorph.

In this paper we complete the study of seminvariants for the various space groups, by considering the non-centrosymmetric space groups for which the conventional unit cell is non-primitive. The non-primitive cell is transformed to an appropriate primitive cell by means of well-known transformations. The methods referred to above are then immediately applicable.

2. Primitive unit cells

The coordinates representing the space group relative to a primitive unit cell are obtained from those corresponding to a non-primitive unit cell (*International Tables*, 1952) by means of the following matrices:

$$C \to P, \quad \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{2·1}$$

$$A \to P, \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \tag{2·2}$$

$$I \to P, \quad \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \tag{2·3}$$

$$F \to P, \quad \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}. \tag{2·4}$$

The results are shown in Table 1.

3. Definitions

In the discussion to follow several concepts will be employed, namely, linear and rational dependence and independence, primitive sets, equivalence and seminvariance. These concepts are defined and developed in our previous papers (Hauptman & Karle, 1956, § 3–§ 7; 1959, § 4 and § 5) to which the reader is referred. They culminate in the main result which identifies the structure seminvariants, namely those linear combinations

$$\sum_{\mathbf{h}} A_{\mathbf{h}} \varphi_{\mathbf{h}}, \tag{3·1}$$

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

$$\sum_{\mathbf{h}} A_{\mathbf{h}} \mathbf{h}_s \equiv 0 \ (\text{mod } \boldsymbol{\omega}_s). \tag{3·2}$$

$\mathbf{h}_s$ is the vector seminvariantly associated with the phase $\varphi_{\mathbf{h}}$, and $\boldsymbol{\omega}_s$ is the seminvariant modulus of the type. The seminvariant vectors and moduli are readily derived from the equivalence classes. These are listed in Table 2. It should be noted that the functional form of the structure factor is the same for all origins comprising an equivalence class.

This paper is concerned with describing in detail simple methods for selecting the origin in each of fourteen types of space groups. The procedures to be presented are of a relatively simple nature, although more general procedures may be readily derived from Table 2.

All the 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 struc-

Table 1. *Coordinates for centered non-centrosymmetric space groups referred to a primitive unit cell*

Space Group						
C2	$X,Y,Z,$	$\bar{Y},\bar{X},\bar{Z}$				
Cm	X,Y,Z	Y,X,Z				
Cc	X,Y,Z	$Y,X,\tfrac{1}{2}+Z$				
Cmm2	X,Y,Z	$\bar{X},\bar{Y},Z,$	$\bar{Y},\bar{X},Z$	Y,X,Z		
$Cmc2_1$	X,Y,Z	$\bar{X},\bar{Y},\tfrac{1}{2}+Z$	$\bar{Y},\bar{X},Z$	$Y,X,\tfrac{1}{2}+Z$		
Ccc2	$X,Y,Z,$	$\bar{X},\bar{Y},Z$	$\bar{Y},\bar{X},\tfrac{1}{2}+Z$	$Y,X,\tfrac{1}{2}+Z$		
C222	X,Y,Z	$\bar{X},\bar{Y},Z$	$\bar{Y},\bar{X},\bar{Z}$	$Y,X,\bar{Z}$		
$C222_1$	X,Y,Z	$\bar{X},\bar{Y},\tfrac{1}{2}+Z$	$\bar{Y},\bar{X},\tfrac{1}{2}+Z$	$Y,X,\bar{Z}$		
Amm2	X,Y,Z	$\bar{X},Y,Z$	X,Z,Y	$\bar{X},Z,Y$		
Abm2	X,Y,Z	$\bar{X},\tfrac{1}{2}+Y,\tfrac{1}{2}+Z$	$X,\tfrac{1}{2}+Z,\tfrac{1}{2}+Y$	$\bar{X},Z,Y$		
Ama2	X,Y,Z	$\tfrac{1}{2}+\bar{X},Y,Z$	$\tfrac{1}{2}+X,Z,Y$	$\bar{X},Z,Y$		
Aba2	X,Y,Z	$\tfrac{1}{2}+\bar{X},\tfrac{1}{2}+Y,\tfrac{1}{2}+Z$	$\tfrac{1}{2}+X,\tfrac{1}{2}+Z,\tfrac{1}{2}+Y$	$\bar{X},Z,Y$		
F432	X,Y,Z $\bar{X}+\bar{Y}+\bar{Z},Z,Y$ $Z,\bar{X}+\bar{Y}+\bar{Z},X$ $Y,X,\bar{X}+\bar{Y}+\bar{Z}$	Z,X,Y $\bar{X}+\bar{Y}+\bar{Z},Y,X$ $Y,\bar{X}+\bar{Y}+\bar{Z},Z$ $X,Z,\bar{X}+\bar{Y}+\bar{Z}$	Y,Z,X $\bar{X}+\bar{Y}+\bar{Z},X,Z$ $X,\bar{X}+\bar{Y}+\bar{Z},Y$ $Z,Y,\bar{X}+\bar{Y}+\bar{Z}$	$\bar{X},\bar{Z},\bar{Y}$ $X+Y+Z,\bar{Y},\bar{Z}$ $\bar{Y},X+Y+Z,\bar{X}$ $\bar{Z},\bar{X},X+Y+Z$	$\bar{Y},\bar{X},\bar{Z}$ $X+Y+Z,\bar{Z},\bar{X}$ $\bar{Z},X+Y+Z,\bar{Y}$ $\bar{X},\bar{Y},X+Y+Z$	$\bar{Z},\bar{Y},\bar{X}$ $X+Y+Z,\bar{X},\bar{Y}$ $\bar{X},X+Y+Z,\bar{Z}$ $\bar{Y},\bar{Z},X+Y+Z$
$F4_132$	$X,Y,Z,$ $X+Y+\bar{Z},Z,Y$ $Z,\bar{X}+\bar{Y}+\bar{Z},X$ $Y,X,\bar{X}+\bar{Y}+\bar{Z}$	Z,X,Y $\bar{X}+\bar{Y}+\bar{Z},Y,X$ $Y,X+\bar{Y}+\bar{Z},Z$ $X,Z,\bar{X}+\bar{Y}+\bar{Z}$	Y,Z,X $\bar{X}+\bar{Y}+\bar{Z},X,Z$ $X,X+\bar{Y}+\bar{Z},Y$ $Z,Y,\bar{X}+\bar{Y}+\bar{Z}$	$\tfrac{1}{4}+\bar{X},\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+\bar{Y}$ $\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{Y},\tfrac{1}{4}+\bar{Z}$ $\tfrac{1}{4}+\bar{Y},\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{X}$ $\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+\bar{X},\tfrac{1}{4}+X+Y+Z$	$\tfrac{1}{4}+\bar{Y},\tfrac{1}{4}+\bar{X},\tfrac{1}{4}+\bar{Z}$ $\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+\bar{X}$ $\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{Y}$ $\tfrac{1}{4}+\bar{X},\tfrac{1}{4}+\bar{Y},\tfrac{1}{4}+X+Y+\bar{Z}$	$\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+\bar{Y},\tfrac{1}{4}+\bar{X}$ $\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{X},\tfrac{1}{4}+\bar{Y}$ $\tfrac{1}{4}+\bar{X},\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{Z}$ $\tfrac{1}{4}+\bar{Y},\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+X+Y+Z.$
F222	X,Y,Z	$Y,X,\bar{X}+\bar{Y}+\bar{Z}$	$\bar{X}+\bar{Y}+\bar{Z},Z,Y$	$Z,\bar{X}+\bar{Y}+\bar{Z},X$		
F23	X,Y,Z $Z,\bar{X}+\bar{Y}+\bar{Z},X$	Z,X,Y $Y,\bar{X}+\bar{Y}+\bar{Z},Z$	Y,Z,X $X,\bar{X}+\bar{Y}+\bar{Z},Y$	$\bar{X}+\bar{Y}+\bar{Z},Z,Y$ $Y,X,\bar{X}+\bar{Y}+\bar{Z}$	$\bar{X}+\bar{Y}+\bar{Z},Y,X$ $X,Z,\bar{X}+\bar{Y}+\bar{Z}$	$\overline{X+Y}+\bar{Z},X,Z$ $Z,Y,\bar{X}+\bar{Y}+\bar{Z}$
$F\bar{4}3m$	X,Y,Z $\bar{X}+\bar{Y}+\bar{Z},Z,Y$ $Z,\bar{X}+\bar{Y}+\bar{Z},X$ $Y,X,\bar{X}+\bar{Y}+\bar{Z}$	Z,X,Y $\bar{X}+\bar{Y}+\bar{Z},Y,X$ $Y,\bar{X}+\bar{Y}+\bar{Z},Z$ $X,Z,\bar{X}+\bar{Y}+\bar{Z}$	Y,Z,X $\bar{X}+\bar{Y}+\bar{Z},X,Z$ $X,\bar{X}+\bar{Y}+\bar{Z},Y$ $Z,Y,\bar{X}+\bar{Y}+\bar{Z}$	X,Z,Y $\bar{X}+\bar{Y}+\bar{Z},Y,Z$ $Y,\bar{X}+\bar{Y}+\bar{Z},X$ $Z,X,\bar{X}+\bar{Y}+\bar{Z}$	Y,X,Z $\bar{X}+\bar{Y}+\bar{Z},Z,X$ $Z,\bar{X}+\bar{Y}+\bar{Z},Y$ $X,Y,\bar{X}+\bar{Y}+\bar{Z}$	Z,Y,X $\bar{X}+\bar{Y}+\bar{Z},X,Y$ $X,\bar{X}+\bar{Y}+\bar{Z},Z$ $Y,Z,\bar{X}+\bar{Y}+\bar{Z}$
$F\bar{4}3c$	X,Y,Z $\bar{X}+\bar{Y}+\bar{Z},Z,Y$ $Z,\bar{X}+\bar{Y}+\bar{Z},X$ $Y,X,\bar{X}+\bar{Y}+\bar{Z}$	Z,X,Y $\bar{X}+\bar{Y}+\bar{Z},Y,X$ $Y,\bar{X}+\bar{Y}+\bar{Z},Z$ $X,Z,\bar{X}+\bar{Y}+\bar{Z}$	Y,Z,X $\bar{X}+\bar{Y}+\bar{Z},X,Z$ $X,\bar{X}+\bar{Y}+\bar{Z},Y$ $Z,Y,\bar{X}+\bar{Y}+\bar{Z}$	$\tfrac{1}{2}+X,\tfrac{1}{2}+Y,\tfrac{1}{2}+Z$ $\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z},\tfrac{1}{2}+Y,\tfrac{1}{2}+Z$ $\tfrac{1}{2}+Y,\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z},\tfrac{1}{2}+X$ $\tfrac{1}{2}+Z,\tfrac{1}{2}+X,\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z}$	$\tfrac{1}{2}+Y,\tfrac{1}{2}+X,\tfrac{1}{2}+Z$ $\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z},\tfrac{1}{2}+Z,\tfrac{1}{2}+X$ $\tfrac{1}{2}+Z,\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z},\tfrac{1}{2}+Y$ $\tfrac{1}{2}+X,\tfrac{1}{2}+Y,\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z}$	$\tfrac{1}{2}+Z,\tfrac{1}{2}+Y,\tfrac{1}{2}+X$ $\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z},\tfrac{1}{2}+X,\tfrac{1}{2}+Y$ $\tfrac{1}{2}+X,\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z},\tfrac{1}{2}+Z$ $\tfrac{1}{2}+Y,\tfrac{1}{2}+Z,\tfrac{1}{2}+\bar{X}+\bar{Y}+\bar{Z}.$
Fmm2	X,Y,Z	$Y,X,\bar{X}+\bar{Y}+\bar{Z}$	$X+Y+Z,\bar{Z},\bar{Y}$	$\bar{Z},X+Y+Z,\bar{X}$		
Fdd2	X,Y,Z	$Y,X,\bar{X}+\bar{Y}+\bar{Z}$	$\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+\bar{Y}$	$\tfrac{1}{4}+\bar{Z},\tfrac{1}{4}+X+Y+Z,\tfrac{1}{4}+\bar{X}$		
Imm2	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$X,X+\bar{Z},X+\bar{Y}$	$Y+\bar{Z},Y,\bar{X}+Y.$		
Iba2	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\tfrac{1}{2}+X,\tfrac{1}{2}+X+\bar{Z},X+\bar{Y}$	$\tfrac{1}{2}+Y+\bar{Z},\tfrac{1}{2}+Y,\bar{X}+Y.$		
Ima2	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$X,\tfrac{1}{2}+X+\bar{Z},\tfrac{1}{2}+X+\bar{Y}$	$Y+\bar{Z},\tfrac{1}{2}+Y,\tfrac{1}{2}+\bar{X}+Y.$		
I222	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\bar{X},\bar{X}+Z,\bar{X}+Y$	$\bar{Y}+Z,\bar{Y},X+\bar{Y}.$		
$I2_12_12_1$	X,Y,Z	$\tfrac{1}{2}+Y+\bar{Z},X+\bar{Z},\tfrac{1}{2}+\bar{Z}$	$\tfrac{1}{2}+\bar{X},\tfrac{1}{2}+\bar{X}+Z,\bar{X}+Y$	$\bar{Y}+Z,\tfrac{1}{2}+\bar{Y},\tfrac{1}{2}+X+\bar{Y}.$		
I4	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$Y,Y+\bar{Z},\bar{X}+Y$	$X+\bar{Z},X,X+\bar{Y}.$		
$I4_1$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\tfrac{3}{4}+Y,\tfrac{1}{4}+Y+\bar{Z},\tfrac{1}{2}+\bar{X}+Y$	$\tfrac{3}{4}+X+\bar{Z},\tfrac{1}{4}+X,\tfrac{1}{2}+X+\bar{Y}.$		
I4mm	X,Y,Z Y,X,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$ $X+\bar{Z},Y+\bar{Z},\bar{Z}$	$Y,Y+\bar{Z},\bar{X}+Y$ $X,X+\bar{Z},X+\bar{Y}$	$X+\bar{Z},X,X+\bar{Y};$ $Y+\bar{Z},Y,\bar{X}+Y.$		

Table 1 (*cont.*)

Space Group				
I4cm	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$Y,Y+\bar{Z},\bar{X}+Y$	$X+\bar{Z},X,X+\bar{Y}$
	$\frac{1}{2}+Y,\frac{1}{2}+X,Z$	$\frac{1}{2}+X+\bar{Z},\frac{1}{2}+Y+\bar{Z},\bar{Z}$	$\frac{1}{2}+X,\frac{1}{2}+X+\bar{Z},X+\bar{Y}$	$\frac{1}{2}+Y+\bar{Z},\frac{1}{2}+Y,\bar{X}+Y$
$I4_1md$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\frac{3}{4}+Y,\frac{1}{4}+Y+\bar{Z},\frac{1}{2}+\bar{X}+Y$	$\frac{3}{4}+X+\bar{Z},\frac{1}{4}+X,\frac{1}{2}+X+\bar{Y}$
	$\frac{3}{4}+Y,\frac{1}{4}+X,\frac{1}{2}+Z$	$\frac{3}{4}+X+\bar{Z},\frac{1}{4}+Y+\bar{Z},\frac{1}{2}+\bar{Z}$	$X,X+\bar{Z},X+\bar{Y}$	$Y+\bar{Z},Y,\bar{X}+Y$
$I4_1cd$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\frac{3}{4}+Y,\frac{1}{4}+Y+\bar{Z},\frac{1}{2}+\bar{X}+Y$	$\frac{3}{4}+X+\bar{Z},\frac{1}{4}+X,\frac{1}{2}+X+\bar{Y}$
	$\frac{1}{4}+Y,\frac{3}{4}+X,\frac{1}{2}+Z$	$\frac{1}{4}+X+\bar{Z},\frac{3}{4}+Y+\bar{Z},\frac{1}{2}+\bar{Z}$	$\frac{1}{2}+X,\frac{1}{2}+X+\bar{Z},X+\bar{Y}$	$\frac{1}{2}+Y+\bar{Z},\frac{1}{2}+Y,\bar{X}+Y$
I422	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$Y,Y+\bar{Z},\bar{X}+Y$	$X+\bar{Z},X,X+\bar{Y}$
	$\bar{Y},\bar{X},\bar{Z}$	$\bar{X}+Z,\bar{Y}+Z,Z$	$\bar{X},\bar{X}+Z,\bar{X}+Y$	$\bar{Y}+Z,\bar{Y},X+\bar{Y}$
$I4_122$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\frac{3}{4}+Y,\frac{1}{4}+Y+\bar{Z},\frac{1}{2}+\bar{X}+Y$	$\frac{3}{4}+X+\bar{Z},\frac{1}{4}+X,\frac{1}{2}+X+\bar{Y}$
	$\bar{Y},\bar{X},\bar{Z}$	$\bar{X}+Z,\bar{Y}+Z,Z$	$\frac{3}{4}+\bar{X},\frac{1}{4}+\bar{X}+Z,\frac{1}{2}+\bar{X}+Y$	$\frac{3}{4}+\bar{Y}+Z,\frac{1}{4}+\bar{Y},\frac{1}{2}+X+\bar{Y}$
$I\bar{4}$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\bar{Y},\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\bar{X}+Y$
$I\bar{4}m2$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\bar{Y},\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\bar{X}+Y$
	$\bar{Y},\bar{X},\bar{Z}$	$\bar{X}+Z,\bar{Y}+Z,Z$	$X,X+\bar{Z},X+\bar{Y}$	$Y+\bar{Z},Y,\bar{X}+Y$
$I\bar{4}c2$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\bar{Y},\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\bar{X}+Y$
	$\frac{1}{2}+\bar{Y},\frac{1}{2}+\bar{X},\bar{Z}$	$\frac{1}{2}+\bar{X}+Z,\frac{1}{2}+\bar{Y}+Z,Z$	$\frac{1}{2}+X,\frac{1}{2}+X+\bar{Z},X+\bar{Y}$	$\frac{1}{2}+Y+\bar{Z},\frac{1}{2}+Y,\bar{X}+Y$
$I\bar{4}2m$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\bar{Y},\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\bar{X}+Y$
	Y,X,Z	$X+\bar{Z},Y+\bar{Z},\bar{Z}$	$\bar{X},\bar{X}+Z,\bar{X}+Y$	$\bar{Y}+Z,\bar{Y},X+\bar{Y}$
$I\bar{4}2d$	X,Y,Z	$Y+\bar{Z},X+\bar{Z},\bar{Z}$	$\bar{Y},\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\bar{X}+Y$
	$\frac{3}{4}+Y,\frac{1}{4}+X,\frac{1}{2}+Z$	$\frac{3}{4}+X+\bar{Z},\frac{1}{4}+Y+\bar{Z},\frac{1}{2}+\bar{Z}$	$\frac{3}{4}+\bar{X},\frac{1}{4}+\bar{X}+Z,\frac{1}{2}+\bar{X}+Y$	$\frac{3}{4}+\bar{Y}+Z,\frac{1}{4}+\bar{Y},\frac{1}{2}+X+\bar{Y}$
I23	X,Y,Z	$\bar{X},\bar{X}+Z,\bar{X}+Y$	$\bar{Y}+Z,\bar{Y},X+\bar{Y}$	$Y+\bar{Z},X+\bar{Z},\bar{Z}$
	Z,X,Y	$\bar{Z},Y+\bar{Z},X+\bar{Z}$	$\bar{X}+Y,\bar{X},\bar{X}+Z$	$X+\bar{Y},\bar{Y}+Z,\bar{Y}$
	Y,Z,X	$\bar{Y},X+\bar{Y},\bar{Y}+Z$	$X+\bar{Z},\bar{Z},Y+\bar{Z}$	$\bar{X}+Z,\bar{X}+Y,\bar{X}$
$I2_13$	X,Y,Z	$\frac{1}{2}+\bar{X},\frac{1}{2}+\bar{X}+Z,\bar{X}+Y$	$\bar{Y}+Z,\frac{1}{2}+\bar{Y},\frac{1}{2}+X+\bar{Y}$	$\frac{1}{2}+Y+\bar{Z},X+\bar{Z},\frac{1}{2}+\bar{Z}$
	Z,X,Y	$\frac{1}{2}+\bar{Z},\frac{1}{2}+Y+\bar{Z},X+\bar{Z}$	$\bar{X}+Y,\frac{1}{2}+\bar{X},\frac{1}{2}+\bar{X}+Z$	$\frac{1}{2}+X+\bar{Y},\bar{Y}+Z,\frac{1}{2}+\bar{Y}$
	Y,Z,X	$\frac{1}{2}+\bar{Y},\frac{1}{2}+X+\bar{Y},\bar{Y}+Z$	$X+\bar{Z},\frac{1}{2}+\bar{Z},\frac{1}{2}+Y+\bar{Z}$	$\frac{1}{2}+\bar{X}+Z,\bar{X}+Y,\frac{1}{2}+\bar{X}$
I432	Coordinates of I23+			
	$\bar{X},\bar{Z},\bar{Y}$	$X,X+\bar{Y},X+\bar{Z}$	$\bar{Y}+Z,Z,\bar{X}+Z$	$Y+\bar{Z},\bar{X}+Y,Y$
	$\bar{Y},\bar{X},\bar{Z}$	$Y,Y+\bar{Z},\bar{X}+Y$	$X+\bar{Z},X,X+\bar{Y}$	$\bar{X}+Z,\bar{Y}+Z,Z$
	$\bar{Z},\bar{Y},\bar{X}$	$Z,\bar{X}+Z,\bar{Y}+Z$	$\bar{X}+Y,Y,Y+\bar{Z}$	$X+\bar{Y},X+\bar{Z},X$
$I4_132$	Coordinates of $I2_13+$			
	$\frac{1}{2}+\bar{X},\frac{1}{2}+\bar{Z},\frac{1}{2}+\bar{Y}$	$X,\frac{1}{2}+X+\bar{Y},X+\bar{Z}$	$\bar{Y}+Z,Z,\frac{1}{2}+\bar{X}+Z$	$\frac{1}{2}+Y+\bar{Z},\bar{X}+Y,Y$
	$\frac{1}{2}+\bar{Y},\frac{1}{2}+\bar{X},\frac{1}{2}+\bar{Z}$	$Y,\frac{1}{2}+Y+\bar{Z},\bar{X}+Y$	$X+\bar{Z},X,\frac{1}{2}+X+\bar{Y}$	$\frac{1}{2}+\bar{X}+Z,\bar{Y}+Z,Z$
	$\frac{1}{2}+\bar{Z},\frac{1}{2}+\bar{Y},\frac{1}{2}+\bar{X}$	$Z,\frac{1}{2}+\bar{X}+Z,\bar{Y}+Z$	$\bar{X}+Y,Y,\frac{1}{2}+Y+\bar{Z}$	$\frac{1}{2}+X+\bar{Y},X+\bar{Z},X$
$I\bar{4}3m$	Coordinates of I23+			
	X,Z,Y	$\bar{X},\bar{X}+Y,\bar{X}+Z$	$Y+\bar{Z},\bar{Z},X+\bar{Z}$	$\bar{Y}+Z,X+\bar{Y},\bar{Y}$
	Y,X,Z	$\bar{Y},\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\bar{X}+Y$	$X+\bar{Z},Y+\bar{Z},\bar{Z}$
	Z,Y,Z	$\bar{Z},X+\bar{Z},Y+\bar{Z}$	$X+\bar{Y},\bar{Y},\bar{Y}+Z$	$\bar{X}+Y,\bar{X}+Z,\bar{X}$
$I\bar{4}3d$	Coordinates of $I2_13+$			
	$\frac{1}{2}+X,\frac{1}{2}+Z,\frac{1}{2}+Y$	$\bar{X}.\frac{1}{2}+\bar{X}+Y,\bar{X}+Z$	$Y+\bar{Z},\bar{Z},\frac{1}{2}+X+\bar{Z}$	$\frac{1}{2}+\bar{Y}+Z,X+\bar{Y},\bar{Y}$
	$\frac{1}{2}+Y,\frac{1}{2}+X,\frac{1}{2}+Z$	$\bar{Y},\frac{1}{2}+\bar{Y}+Z,X+\bar{Y}$	$\bar{X}+Z,\bar{X},\frac{1}{2}+\bar{X}+Y$	$\frac{1}{2}+X+\bar{Z},Y+\bar{Z},\bar{Z}$
	$\frac{1}{2}+Z,\frac{1}{2}+Y,\frac{1}{2}+X$	$\bar{Z},\frac{1}{2}+X+\bar{Z},Y+\bar{Z}$	$X+\bar{Y},\bar{Y},\frac{1}{2}+\bar{Y}+Z$	$\frac{1}{2}+\bar{X}+Y,\bar{X}+Z,\bar{X}$

ture-factor magnitudes is given (so that, for a fixed functional form of the structure factor, the magnitudes of all the structure seminvariants are determined) and the sign of any one structure seminvariant, the magnitude of which is different from 0 or π, has been arbitrarily specified.

It is further assumed throughout this paper that the functional form of the structure factor is fixed.

4. The remaining types of space groups

4·01. *Type* $2P_002$

Theorem 4·01·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant, i.e. its value is uniquely determined if, and only if, $h=k$ and l is even.

Theorem 4·01·2. Let $h_1=k_1$. Then any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. l_1 is odd) has

Table 2. *Equivalence classes, seminvariant vectors and seminvariant moduli for the centered non-centrosymmetric space groups, referred to a primitive unit cell*

Category	2							3						4
No. of equivalence classes	2							4						8
Type	$2P_002$	2P00	2P20	2P22	$2P_120$	$2P_1022$	$2P_1222$	$3P_22$	$3P_24$	$3P_30$	$3P_32$	$3P_34$	$3P_40$	4P111
Space groups	C2	Cm Cc	Cmm2 $Cmc2_1$ Ccc2	C222 $C222_1$	Amm2 Abm2 Ama2 Aba2	Imm2 Iba2 Ima2	I222 $I2_12_12_1$	F432 $F4_132$	F222 F23 $F\bar{4}3m$ $F\bar{4}3c$	I4 $I4_1$ I4mm I4cm $I4_1md$ $I4_1cd$	I422 $I4_122$	$I\bar{4}$ $I\bar{4}m2$ $I\bar{4}c2$ $I\bar{4}2m$ $I\bar{4}2d$	Fmm2 Fdd2	I23 $I2_13$ I432 $I4_132$ $I\bar{4}3m$ $I\bar{4}3d$
Equivalence classes of origins	[Y, $\bar{Y}$, 0 Y, $\bar{Y}$, ½] [Y, ½+$\bar{Y}$, 0 Y, ½+$\bar{Y}$, ½]	[X, X, Z] [X, ½+X, Z]	[0, 0, Z ½, ½, Z] [0, ½, Z ½, 0, Z]	[0, 0, 0 0, 0, ½ ½, ½, 0 ½, ½, ½] [½, 0, 0 ½, 0, ½ 0, ½, 0 0, ½, ½]	[0, X, X ½, X, X] [0, X, ½+X ½, X, ½+X]	[Z, Z, 0 Z, ½+Z, ½] [Z, Z, ½ Z, ½+Z, 0]	[0, 0, 0 ½, ½, 0 ½, 0, ½ 0, ½, ½] [½, 0, 0 0, ½, 0 0, 0, ½ ½, ½, ½]	[0, 0, 0 ½, ½, ½] [½, 0, 0 0, ½, ½] [0, ½, 0 ½, 0, ½] [0, 0, ½ ½, ½, 0]	[0, 0, 0 ¼, ¼, ¼ ½, ½, ½ ¾, ¾, ¾] [0, ½, 0 ¼, ¾, ¼ ½, 0, ½ ¾, ¼, ¾] [½, 0, 0 ¾, ¼, ¼ 0, ½, ½ ¼, ¾, ¾] [0, 0, ½ ¼, ¼, ¾ ½, ½, 0 ¾, ¾, ¼]	[Z, Z, 0] [Z, Z, ½] [Z, ½+Z, 0] [Z, ½+Z, ½]	[0, 0, 0 ½, ½, 0] [½, 0, 0 0, ½, 0] [0, 0, ½ ½, ½, ½] [½, 0, ½ 0, ½, ½]	[0, 0, 0 ½, ½, 0 ¼, ¾, ½ ¾, ¼, ½] [0, 0, ½ ½, ½, ½ ¼, ¾, 0 ¾, ¼, 0] [½, 0, 0 0, ½, 0 ¾, ¾, ½ ¼, ¼, ½] [½, 0, ½ 0, ½, ½ ¾, ¾, 0 ¼, ¼, 0]	[Z, Z, $\bar{Z}$] [½+Z, Z, $\bar{Z}$] [Z, ½+Z, $\bar{Z}$] [Z, Z, ½+$\bar{Z}$]	[0, 0, 0] [½, 0, 0] [0, ½, 0] [0, 0, ½] [½, ½, 0] [½, 0, ½] [0, ½, ½] [½, ½, ½]
Seminvariant vector	(h − k, l)	(h + k, l)			(h, k + l)	(h + k, k + l, l + h)		(h + k + l)		(h + k)		(h − k + 2l)	(h + k − l)	(h, k, l)
Seminvariant modulus	(0, 2)	(0, 0)	(2, 0)	(2, 2)	(2, 0)	(0, 2, 2)	(2, 2, 2)	(2)	(4)	(0)	(2)	(4)	(0)	(1, 1, 1)
Seminvariant phases	φ_{llg}	$\varphi_{l\bar{l}0}$	φ_{gg0}, φ_{uu0}	φ_{ggg}, φ_{uug}	φ_{ghh}	$\varphi_{h\bar{h}l}$ h l (mod 2)	φ_{ggg}, φ_{uuu}	φ_{ggg}, φ_{uug}, φ_{ugu}, φ_{guu}	φ_{hkl} $h + k + l = 0$ (mod 4)	$\varphi_{h\bar{h}l}$	φ_{ggl}, φ_{uul}	φ_{hkl}, $h - k = 2l$ (mod 4)	$\varphi_{h,k,h+k}$	φ_{hkl}
No. of phases, lin. semi-ind., to be specified	2							1						0

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. $h=k$) is uniquely determined.

Theorem 4·01·3. Let l_2 be even. Then the value of any phase $\varphi_{\mathbf{h}_2}$ which is linearly semi-independent (i.e. $h_2-k_2\neq 0$) may be specified arbitrarily. Once this is done, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_2}$ (i.e. l is even and $h-k$ is divisible by h_2-k_2) is uniquely determined. 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 $h_2-k_2=\pm 1$.

Theorem 4·01·4. Let $h_1=k_1$ and l_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. l_1 is odd and $h_2-k_2=0$). In accordance with the two previous theorems, 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 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. 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 $h_2-k_2=\pm 1$.

4·02. *Type* 2*P*00

Theorem 4·02·1. A single phase $\varphi_{\mathbf{h}}$ is a structure seminvariant, i.e. its value is uniquely determined, if, and only if, $h+k=l=0$.

Theorem 4·02·2. The value of any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. h_1+k_1 and l_1 are not both zero) may be specified arbitrarily. Once this is done, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined. Any phase $\varphi_{\mathbf{h}}$ which is 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 the greatest common divisor of h_1+k_1 and l_1 is unity.

Theorem 4·02·3. The values of any two phases $\varphi_{\mathbf{h}_1}, \varphi_{\mathbf{h}_2}$, constituting a linearly semi-independent set, i.e.

$$\begin{vmatrix} h_1+k_1 & l_1 \\ h_2+k_2 & l_2 \end{vmatrix} \neq 0\,,$$

may be specified arbitrarily. Once this is done, 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. 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

$$\begin{vmatrix} h_1+k_1 & l_1 \\ h_2+k_2 & l_2 \end{vmatrix} = \pm 1\,.$$

4·03. *Type* 2*P*20

4·04. *Type* 2*P*22

These types have been treated previously (Hauptman & Karle, 1956).

4·05. *Type* 2*P*$_1$20

Theorem 4·05·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, h is even and $k+l=0$.

Theorem 4·05·2. Let $k_1+l_1=0$. Then any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. h_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, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ (i.e. $k+l=0$) is uniquely determined.

Theorem 4·05·3. Let h_2 be even. Then the value of any phase $\varphi_{\mathbf{h}_2}$ which is linearly semi-independent (i.e. $k_2+l_2=0$) may be specified arbitrarily. Once this is done, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_2}$ is uniquely determined. 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 $k_2+l_2=\pm 1$.

Theorem 4·05·4. Let $k_1+l_1=0$ and h_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 is odd and $k_2+l_2\neq 0$). In accordance with the two previous theorems 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, 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. 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 $k_2+l_2=\pm 1$.

4·06. *Type* 2*P*$_1$022

Theorem 4·06·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h+k=0$ and $h\equiv l$ (mod 2).

Theorem 4·06·2. Let $h_1+k_1=0$. Then any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-independent (i.e. h_1+l_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, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Theorem 4·06·3. Let $h_2+k_2\neq 0$, so that $\varphi_{\mathbf{h}_2}$ is linearly semi-independent. Then the value of $\varphi_{\mathbf{h}_2}$ may be specified arbitrarily. Once this is done, the value of any phase $\varphi_{\mathbf{h}}$, which is linearly semi-dependent on $\varphi_{\mathbf{h}_2}$, is uniquely determined. Any phase $\varphi_{\mathbf{h}}$ which is rationally semi-dependent on $\varphi_{\mathbf{h}_2}$ is also linearly semi-dependent on $\varphi_{\mathbf{h}_2}$ provided that $\varphi_{\mathbf{h}_2}$ is semi-primitive, i.e. provided that $h_2+k_2=\pm 1$.

Theorem 4·06·4. Choose $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ as in the previous two theorems. In accordance with these theorems either of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen and the value of $\varphi_{\mathbf{h}_2}$ may be specified arbitrarily. Once this is done 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 $h_2+k_2=\pm 1$.

4·07. *Type* $2P_1222$

Theorem 4·07·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h\equiv k\equiv l \pmod 2$.

Theorem 4·07·2. Any phase $\varphi_{\mathbf{h}_1}$ which is linearly semi-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 the value of any phase which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

Theorem 4·07·3. Let the pair of phases $\varphi_{\mathbf{h}_1}$, $\varphi_{\mathbf{h}_1}$, be a linearly semi-independent set. In accordance with the previous theorem, either of the two possible values of $\varphi_{\mathbf{h}_1}$ may be chosen and either of the two possible values of $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done, 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.

4·08. *Type* $3P_22$

This type has been previously described (Hauptman & Karle, 1956).

4·09. *Type* $3P_24$

Theorem 4·09·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h+k+l\equiv 0 \pmod 4$.

Theorem 4·09·2. Let the phase $\varphi_{\mathbf{h}_1}$ be linearly semi-independent. Depending upon whether $h_1+k_1+l_1$ is odd or even, there are four or two possible values for $\varphi_{\mathbf{h}_1}$ (differing by $\pi/2$ or π respectively).

In the first case any of the four possible values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_1}$, is uniquely determined.

In the second case either of the two possible 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 $\varphi_{\mathbf{h}_1}$ is uniquely determined. Furthermore any phase $\varphi_{\mathbf{h}_2}$ which is linearly semi-independent of $\varphi_{\mathbf{h}_1}$ then has two possible values differing from each other by π. Either one of these two values for a particular such phase $\varphi_{\mathbf{h}_2}$ may be chosen. Once this is done the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_2}$, is uniquely determined.

4·10. *Type* $3P_30$

Theorem 4·10·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h+k=0$.

Theorem 4·10·2. Let $h_1+k_1\neq 0$, so that $\varphi_{\mathbf{h}_1}$ is linearly semi-independent. Then the value of $\varphi_{\mathbf{h}_1}$ may be specified arbitrarily. Once this is done, 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 $\varphi_{\mathbf{h}_1}$, provided that $\varphi_{\mathbf{h}_1}$ is semi-primitive, i.e. provided that $h_1+k_1=\pm 1$.

4·11. *Type* $3P_32$*

Theorem 4·11·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h+k$ is even.

Theorem 4·11·2. Let h_1+k_1 be odd so that $\varphi_{\mathbf{h}_1}$ is linearly semi-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 may be chosen. Once this is done, the value of any phase, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined.

4·12. *Type* $3P_34$

Theorem 4·12·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h-k\equiv 2l \pmod 4$.

Theorem 4·12·2. Let the phase $\varphi_{\mathbf{h}_1}$ be linearly semi-independent. Depending upon whether $h_1-k_1+2l_1$, is odd or even, there are four or two possible values for $\varphi_{\mathbf{h}_1}$ (differing by $\pi/2$ or π, respectively).

In the first case any of the four possible values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done, the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_1}$, is uniquely determined.

In the second case either of the two possible values for $\varphi_{\mathbf{h}_1}$ may be chosen. Once this is done, the value of any phase $\varphi_{\mathbf{h}}$ which is linearly semi-dependent on $\varphi_{\mathbf{h}_1}$ is uniquely determined. Furthermore any phase $\varphi_{\mathbf{h}_2}$ which is linearly semi-independent of $\varphi_{\mathbf{h}_1}$, then has two possible values differing from each other by π. Either one of these two values, for a particular such phase $\varphi_{\mathbf{h}_2}$, may be chosen. Once this is done the value of any phase $\varphi_{\mathbf{h}}$, of necessity linearly semi-dependent on $\varphi_{\mathbf{h}_2}$, is uniquely determined.

4·13. *Type* $3P_40$

Theorem 4·13·1. A single phase $\varphi_{\mathbf{h}}$ is a seminvariant if, and only if, $h+k=l$.

Theorem 4·13·2. Let $h_1+k_1-l_1\neq 0$, so that $\varphi_{\mathbf{h}_1}$ is linearly semi-independent. Then the value of $\varphi_{\mathbf{h}_1}$ may be specified arbitrarily. Once this is done, 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 $\varphi_{\mathbf{h}_1}$, provided that $\varphi_{\mathbf{h}_1}$ is semi-primitive, i.e. provided that $h_1+k_1-l_1=\pm 1$.

4·14. *Type* $4P111$

Theorem 4·14·1. Every phase is a seminvariant.

* For space group $P(I4_122)$, the signs of all seminvariants are uniquely determined. In this case, therefore, the specification of the sign of a seminvariant is not a requirement for theorems 4·11·1 and 4·11·2 to be valid.

5. Concluding remarks

This paper concludes the study of the seminvariants for the non-centrosymmetric space groups which was initiated in a previous paper (Hauptman & Karle, 1956). The theory of the seminvariants provides a basis for specifying an origin and the enantiomorph or reference frame when required. Furthermore it demonstrates the existence of relationships between the measured intensities and the values of phases. It will be the purpose of future publications to elucidate the exact nature of these relationships and by these means to continue the unified program for phase determination in the non-centrosymmetric space groups which has already been completed for the centrosymmetric ones (Karle & Hauptman, 1961 ff.).

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Neutron Diffraction Investigation of Solid Solutions $AlTh_2D_n$

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Solid solutions of composition $AlTh_2D_n$, with $n = 0, 2, 3, 4$, have been studied by means of neutron diffraction. For $n = 4$ the deuterium atoms completely fill a set of equivalent Th-tetrahedra, quite similar to the arrangement in thorium hydride. For the other compositions these sites are partly occupied. No evidence for ordering has been found, even at a temperature of 82 °K.

The intermetallic compound $AlTh_2$ easily absorbs hydrogen. Apart from a two-phase region at room temperature between the compositions $AlTh_2H_0$ and $AlTh_2H_{\sim 1.5}$, the hydrogen is dissolved homogeneously until the ultimate composition $AlTh_2H_4$ is reached (van Vucht, 1960). X-ray investigation shows that the tetragonal symmetry of $AlTh_2$ is conserved in the solid solutions. When the lattice parameters are plotted against n, the number of hydrogen atoms per $AlTh_2$, a is found to increase up to $n = 2$. There it shows a sharp break, followed by a decrease until saturation. On the other hand c increases monotonically.

As part of a larger program, a neutron-diffraction investigation was undertaken with the object of establishing the hydrogen positions. Only microcrystalline samples were available so that to avoid a large background of incoherent scattering the deuterides rather than hydrides were used. The relevant neutron scattering lengths (Shull & Wollan, 1956) are, in 10^{-12} cm., $b_{Al} = 0.35$, $b_{Th} = 1.01$ and $b_D = 0.65$.

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Experimental procedure

The deuterides were prepared in exactly the same way as the hydrides (van Vucht, 1960). For the room-temperature neutron-diffraction measurements 10 mm. dia. cylindrical thin-walled aluminium sample holders were used. By means of a glass tube and a section of fernico tube these were connected to the apparatus in which the deuteride was prepared. Using a tilting arrangement the finished product could be transferred to the sample holder under vacuum after which the glass connecting tube was sealed off. The sample holder was then placed on the diffractometer described by Goedkoop (1957) and the diffraction pattern recorded with 1·026 Å neutrons. Resolution was mainly determined by Soller slits 0·25 mm. wide and 200 mm. long placed in front of the counter.

For measurements at low temperature a single-jacketed vacuum cryostat as shown in Fig. 1 was placed on the goniometer. Liquid air or liquid nitrogen was placed in the inner cylinder, to the bottom of which the sample holder was fixed. The glass-sealed sample holders were unsuited for this arrangement and so a shorter one closed by means of a screw-plug