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Seminvariant vectors for centred space groups. By S. R. HALL, *Crystallography Centre, University of Western Australia, Nedlands, WA* 6009, *Australia*

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Abstract

Existing tables of seminvariant vectors for centred spacegroups are in terms of primitive indices only. The seminvariant vectors for use with centred indices are derived and tabulated for centred spacegroups.

The origin of a cell may be fixed by specifying the structure-factor phases of a prescribed number of linearly independent reflections (Hauptman & Karle, 1953). For a given space group certain reflections are ineligible for this purpose because their phase values are independent of the cell origin. These phases are known as structure seminvariants (Hauptman & Karle, 1953). The two properties that characterize structure seminvariants are the seminvariant vectors **V** and the seminvariant moduli **m** (Hauptman & Karle, 1956). Tables of **V** and **m** appear in Hauptman & Karle (1959), Karle & Hauptman (1961) and § 6.1 of *International Tables for X-ray Crystallography* (1974).

For centred space groups these tables list the seminvariant vectors **V** in terms of primitive indices. This has led to the practice in direct methods of transforming the indices of centred space groups into their primitive form, and selecting the reflections to fix the origin of the primitive cell. A more computationally convenient approach is to transform the primitive seminvariant vectors into the centred equivalent and use these directly with centred indices.

The procedures for applying the primitive seminvariant vectors $\mathbf{V}_p$ and moduli **m** to identify seminvariant reflections are based on the transformed indices $\mathbf{h}'$:

$$\mathbf{h}' = \mathbf{V}_p \mathbf{h}_p, \tag{1}$$

where $\mathbf{V}_p$ is the primitive seminvariant vector set (see Tables 2 and 3) and $\mathbf{h}_p$ are the primitive indices. A single phase is a structure seminvariant if

$$\mathbf{h}' \ (\mathrm{mod}\ \mathbf{m}) \equiv 0. \tag{2}$$

For centred space groups the centred indices $\mathbf{h}_c$ are converted to primitive indices $\mathbf{h}_p$ by the transformation

$$\mathbf{h}_p = \mathbf{T}\mathbf{h}_c, \tag{3}$$

Table 1. *Centred to primitive cell transformation matrices* **T**

A	*C*	*I*	*F*
$\begin{matrix}-1 & 0 & 0\\ 0 & -\frac{1}{2} & \frac{1}{2}\\ 0 & \frac{1}{2} & \frac{1}{2}\end{matrix}$	$\begin{matrix}\frac{1}{2} & \frac{1}{2} & 0\\ \frac{1}{2} & -\frac{1}{2} & 0\\ 0 & 0 & -1\end{matrix}$	$\begin{matrix}-\frac{1}{2} & \frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2}\end{matrix}$	$\begin{matrix}0 & \frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & 0 & \frac{1}{2}\\ \frac{1}{2} & \frac{1}{2} & 0\end{matrix}$

Table 2. *Seminvariant vectors and moduli for the centrosymmetric centred space groups*

To be used in conjunction with *International Tables for X-ray Crystallography* (1974, § 6.1).

Type	$2P$	$2P_1$	$3P_2$	$3P_3$	$4P$
Centre	*C*	*I*	*F*	*I*	*I*
$\mathbf{V}_p$	1 1 0	0 1 1	1 1 1	1 1 0	0 0 0
	0 0 1	1 0 1	0 0 0	0 0 0	0 0 0
	0 0 0	1 1 0	0 0 0	0 0 0	0 0 0
	$h+k, l$	$h+k, k+l, l+h$	$h+k+l$	$h+k$	—
$\mathbf{V}_c$	1 0 0	1 0 0	1 1 1	0 0 1	0 0 0
	0 0 1	0 1 0	0 0 0	0 0 0	0 0 0
	0 0 0	0 0 1	0 0 0	0 0 0	0 0 0
	h, l	h, k, l	$h+k+l$	l	—
m	2,2	2,2,2	2	2	—

Table 3. *Seminvariant vectors and moduli for the noncentrosymmetric centred space groups*

To be used in conjunction with *International Tables for X-ray Crystallography* (1974, § 6.1).

Types	$2P_02$	$2P00$ $2P20$ $2P22$	$2P_120$	$2P_1022$ $2P_1222$	$3P_22$ $3P_24$	$3P_30$ $3P_32$	$3P_34$	$3P_40$	$4P111$
Centre	*C*	*C*	*A*	*I*	*F*	*I*	*I*	*F*	*I*
$\mathbf{V}_p$	1 −1 0	1 1 0	1 0 0	0 1 1	1 1 1	1 1 0	1 −1 2	1 1 −1	0 0 0
	0 0 1	0 0 1	0 1 1	1 0 1	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
	0 0 0	0 0 0	0 0 0	1 1 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
	$h-k, l$	$h+k, l$	$h, k+l$	$h+k, k+l, l+h$	$h+k+l$	$h+k$	$h-k+2l$	$h+k-l$	—
$\mathbf{V}_c$	0 1 0	1 0 0	1 0 0	1 0 0	1 1 1	0 0 1	0 2 −1	0 0 1	0 0 0
	0 0 1	0 0 1	0 0 1	0 1 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
	0 0 0	0 0 0	0 0 0	0 0 1	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
	k, l	h, l	h, l	h, k, l	$h+k+l$	l	$2k-l$	l	—
m	0,2	0,0 2,0 2,2	2,0	0,2,2 2,2,2	2 4	0 2	4	0	—

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where **T** is one of the cell transformation matrices listed in Table 1. Substituting (3) into (1) we obtain

$$\mathbf{h}' = \mathbf{V}_p \mathbf{T} \mathbf{h}_c \quad (4)$$

$$\mathbf{h}' = \mathbf{V}_c \mathbf{h}_c, \quad (5)$$

where $\mathbf{V}_c$ is the centred seminvariant vector matrix listed in Table 2 for centrosymmetric space groups and in Table 3 for noncentrosymmetric space groups. The seminvariant moduli **m** are unaltered by this transformation. These $\mathbf{V}_c$ matrices provide the means to derive the seminvariant indices **h**′ directly from the centred indices. This approach is already in use in direct-methods software (Hall, 1982).

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