Acta Cryst. (1979). A**35**, 733–745

On Equivalent Subgroups and Supergroups of the Space Groups

By E. F. Bertaut

Laboratoire de Cristallographie, CNRS 166 *X*, 38042 *Grenoble CEDEX, France*

and Y. Billiet

Laboratoire de Chimie Inorganique Moléculaire, 6, *avenue Le Gorgeu*, 29283 *Brest, France*

(*Received* 14 *November* 1978; *accepted* 5 *March* 1979)

Abstract

Symmetry operators $(\alpha|\tau_\alpha)$ of a space group G and $(\beta|\tau_\beta)$ of a subgroup g are conjugated with respect to a similarity operator $\mathsf{S} = (\mathbf{S}|\mathbf{T})$ where $\mathbf{S}$ is a 3×3 matrix and $\mathbf{T}$ a column matrix. The matrix $\mathbf{S}$ relates the lattice vectors of G to those of g whilst $\mathbf{T}$ describes the origin of the lattice of g in the coordinate system of G. We determine here the coefficients of the matrix $\mathbf{S}$ when G and g are equivalent, *i.e.* isosymbolic or enantiomorphic. Here the index of g in G is equal to $|\det \mathbf{S}|$. Its lowest values are tabulated for all space groups.

1. Introduction and outline

One of the authors (Billiet, 1973) has shown that each space group G referred to a unit cell **A**, **B**, **C** and an origin O has an infinity of subgroups g having the same Hermann–Mauguin space group symbol, but an increased unit cell **a**, **b**, **c** at the origin o. Such subgroups g with the same symbol as G were called 'isosymbolic'. **a**, **b**, **c** and **A**, **B**, **C** are related by the equation

$$(\mathbf{a},\mathbf{b},\mathbf{c}) = (\mathbf{A},\mathbf{B},\mathbf{C})\mathbf{S}. \quad (1)$$

Here (**a**,**b**,**c**) and (**A**,**B**,**C**) are row matrices and **S** is a 3×3 matrix; its coefficients s_{ij} are integers.* The coefficients of the matrix **S** as well as the coordinates of the origin o were found by a direct mapping procedure of the coordinate triplets of the Wyckoff families of g onto G as described in the reference above. We choose here an analytical procedure which relates **S** to the specific symmetry operations by an important conjugation relation.

The determinant of **S** is abbreviated det **S**; its modulus is equal to the index of g in G and represents the volume ratio of **abc** and **ABC**. In previous work (Billiet, 1973) it was restricted to positive values which means that the 'handedness' of G was conserved in g.

* The coefficients s_{ij} are always integer numbers when g is an equivalent subgroup of G.

We consider here the general case where det **S** may be positive as well as negative. It is well known that a screw axis 3_1 is changed into a 3_2 axis by a change of handedness. Thus we consider not only the isosymbolic, but also the enantiomorphic groups. This is the reason why we have chosen the title of equivalent subgroups for those subgroups g which are either isosymbolic or enantiomorphic with G.

2. The conjugation relation

The proof given here is valid for the most general form of **S**, for s_{ij} integral or not, also when g is a non-equivalent subgroup of G,* say. $\mathbf{R}(X,Y,Z)$ and $\mathbf{r}(x,y,z)$ are column matrices in G and g respectively, described by the conventional crystallographic coordinates. If **T** is the column matrix X_o, Y_o, Z_o which describes the origin o of the reference system $(o,\mathbf{a},\mathbf{b},\mathbf{c})$ of g in the coordinate system of G, one has

$$\mathbf{R} = \mathbf{T} + \mathbf{S}\mathbf{r}. \quad (2)$$

If $(\alpha|\tau_\alpha)$ is a symmetry operator in G, one has

$$\mathbf{R}' = (\alpha|\tau_\alpha)\mathbf{R} = \alpha\mathbf{R} + \tau_\alpha. \quad (3)$$

Similarly, if $(\beta|\tau_\beta)$ is the homologous† symmetry operator in g, one has (see Fig. 1)

$$\mathbf{r}' = (\beta|\tau_\beta)\mathbf{r} = \beta\mathbf{r} + \tau_\beta. \quad (4)$$

Between **R**′ and **r**′ one has the relation

$$\mathbf{R}' = \mathbf{T} + \mathbf{S}\mathbf{r}'. \quad (5)$$

In (3), replacing **R**′ and **R** by their expressions given in (5) and (2), respectively, one has

$$\mathbf{S}\mathbf{r}' = \alpha\mathbf{S}\mathbf{r} + [\alpha - (\mathbf{1})]\mathbf{T} + \tau_\alpha. \quad (6)$$

Multiplying (4) by **S** and identifying with (6) we obtain the important relation between operators

$$(\mathbf{S}|\mathbf{T})\,(\beta|\tau_\beta) = (\alpha|\tau_\alpha)\,(\mathbf{S}|\mathbf{T}), \quad (C)$$

* See previous footnote.

† Two symmetry operators $(\alpha|\tau_\alpha)$ and $(\beta|\tau_\beta)$ are homologous if they represent the *same operation in space*, but are expressed in the (different) coordinate systems of G and g, $(O,\mathbf{A},\mathbf{B},\mathbf{C})$ and $(o,\mathbf{a},\mathbf{b},\mathbf{c})$, respectively.

0567-7394/79/050733-13$01.00

which, separating the rotational and translational parts, splits into

$$\mathbf{S}\beta = \alpha\mathbf{S}, \quad (7)$$

$$\mathbf{S}\tau_\beta = \tau_\alpha + [\alpha - (\mathbf{1})]\mathbf{T}. \quad (8)$$

Here $(\mathbf{1})$ is the unit matrix. We rewrite the last equation in the following more convenient form, restricting $\hat{\tau}_\alpha$ to be less than a lattice translation t_G in G by the usual convention $\tau = \hat{\tau} + t$,

$$\mathbf{S}\hat{\tau}_\beta - \hat{\tau}_\alpha + [(\mathbf{1}) - \alpha]\mathbf{T} = t_G. \quad (8a)$$

Relations (7) and (8*a*) determine the matrix **S** and the vector **T**, say the unit cell in g, its magnitude and position.

Remark

The basic relation above has been called (C) to recall that it expresses a *conjugation*: the operators $\mathsf{a} = (\alpha|\tau_\alpha)$ of G and $\mathsf{b} = (\beta|\tau_\beta)$ of g are conjugated with respect to the similarity operator

$$\mathsf{S} = (\mathbf{S}|\mathbf{T}),$$

$$\mathsf{b} = \mathsf{S}^{-1}\,\mathsf{a}\mathsf{S}. \quad (C')$$

Also, (C) is more general than stated here and applies to *any* group–subgroup relation. Similarities include symmetries as special cases and we shall discuss in another paper the group of similarity operators. Note that our definition of equivalent subgroups implies $|\det \mathbf{S}| \geq 1$, thus including the case $|\det \mathbf{S}| = 1$ which corresponds to the automorphisms of G.

We shall first discuss two special cases, those of pure lattice translations and of symmorphic space groups.

2.1. *Pure translations*

The operators $(\alpha|\tau_\alpha)$ and $(\beta|\tau_\beta)$ can be represented by $(1|t_G)$ and $(1|t_g)$ respectively and relation (C) reduces to

$$\mathbf{S}t_g = t_G. \quad (8b)$$

The case of centred lattices (8*b*) introduces parity rules for the coefficients s_{ij} of **S** as will be shown later.

2.2. *Symmorphic space groups and choice of origin*

If G and g are symmorphic space groups, the operators of their generators $(\alpha|\tau_\alpha)$ and $(\beta|\tau_\beta)$ can be chosen such that $\tau_\alpha = \tau_\beta \equiv 0$ and (8*a*) simplifies to

$$[(\mathbf{1}) - \alpha]\mathbf{T} = t_G. \quad (8c)$$

This relation *does not contain* **S** and thus expresses a fundamental property of the symmetry operator $(\alpha|000)$ in the group G. The solution of (8*c*) corresponds to the location **T** of the symmetry elements equivalent to α. The solutions $\mathbf{T}_i$ of (8*c*) for the generators $(\alpha_i|000)$ of G have an intersection which forms the set of possible origins of g. We give some examples when α corresponds to $\bar{1}$, 4, $\bar{4}$, 2_x and 3 in Appendix A.

2.3. *Remark*

If the origin is chosen on a screw axis or glide plane corresponding to the operator $(\alpha|\hat{\tau}_\alpha)(\hat{\tau}_\alpha \neq 0)$, the solution of (8*c*) still indicates the locations **T** of the equivalent symmetry elements. This suggests the following 'decoupling procedure'. If one finds consistent solutions

$$\mathbf{S}\hat{\tau}_\beta - \hat{\tau}_\alpha = t_G \quad and \quad [(\mathbf{1}) - \alpha]\,\mathbf{T} = t'_G, \quad (8d)$$

then (8*a*) is certainly verified. We have applied this procedure in the discussion of $I4_1/a$ (see § 4.4.1). This procedure is also allowed for $\mathbf{T} = \mathbf{0}$, *i.e.* for the same choice of origins in G and g where (8*d*) reduces to

$$\mathbf{S}\hat{\tau}_\beta - \hat{\tau}_\alpha = t_G. \quad (8e)$$

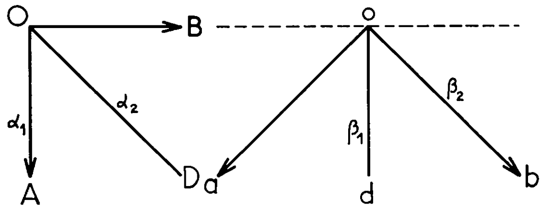

Fig. 1. Homologous symmetry operators. The left and right parts correspond to G and g respectively. If $\alpha_1 = 2_x$ is the operator of a twofold rotation about OA, the homologous operator in g is $\beta_1 = 2_{xx}$ [see equations (12)] in the example $P422$ of the text. In the same way, if $\alpha_2 = 2_{xx}$ is the operator of a twofold rotation about the diagonal OD, the homologous operator in g is $\beta_2 = 2_y$. The same figure provides the illustration for the 'class equivalent' space groups considered in Appendix B where $\alpha_1 = m_x$ is the operation of a mirror perpendicular to OA and $\beta_1 = m_{xx}$ is that of a mirror perpendicular to the line od and transforming x,y,z to $\bar{y},\bar{x},z$.

3. Form of the matrix S

3.1. *Tetragonal, hexagonal, trigonal, rhombohedral and monoclinic groups*

We shall derive the form of **S** for tetragonal, hexagonal, trigonal, rhombohedral and monoclinic groups. The principal axis is taken along Oz with the same orientation in G and g. The matrix expressions of α and β are then formally the same.* As a consequence (*cf.* 7), $\alpha = \beta$ commutes with **S**.

* One may also study the case of $\beta = \alpha^{-1}$ (opposite orientation), but it does not introduce new features.

3.1.1. *Tetragonal.* Here

$$\alpha = \mathbf{4} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad (9)$$

$$\mathbf{S} \times \mathbf{4} = \begin{bmatrix} s_{12} & -s_{11} & s_{13} \\ s_{22} & -s_{21} & s_{23} \\ s_{32} & -s_{31} & s_{33} \end{bmatrix} = \mathbf{4} \times \mathbf{S} = \begin{bmatrix} -s_{21} & -s_{22} & -s_{23} \\ s_{11} & s_{12} & s_{13} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}. \qquad (7')$$

The identification of the coefficients leads to the relations $s_{11} = s_{22}$; $s_{12} = -s_{21}$; $s_{13} = s_{23} = s_{31} = s_{32} = 0$. Thus in the tetragonal system, **S** has the general form

$$\mathbf{Q}_1 = \begin{bmatrix} s_{11} & -s_{21} & 0 \\ s_{21} & s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}. \qquad (10a)$$

This is also the only form for those tetragonal space groups which belong to the classes 4, $\bar{4}$, and $4/m$.

$$\det \mathbf{Q}_1 = s_{33}(s_{11}^2 + s_{21}^2). \qquad (11)$$

For all other tetragonal space groups, s_{21} takes special values. When the supplementary symmetry elements (mirrors parallel or/and binary axes perpendicular to the fourfold axis) have the same orientation in G and g, their rotational parts commute with **S**, implying

$$s_{21} = 0$$

and

$$\mathbf{Q}_2 = \mathbf{Q}_1(s_{21} = 0) = \begin{bmatrix} s_{11} & 0 & 0 \\ 0 & s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}. \qquad (10b)$$

When the last two (binary) symmetry elements of the HM (Hermann–Mauguin) symbol are identical, other orientations are allowed. For instance, in $P422$ the identical orientation leads to $\mathbf{Q}_2$, but the following orientation is also possible with the 2_x axis in g rotated by 45° with respect to the 2_x axis in G so that (*cf.* Fig. 1)

$$\beta = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \mathbf{2}_{xx}, \quad \alpha = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \mathbf{2}_x. \qquad (12)$$

From $\mathbf{Q}_1\beta = \alpha\mathbf{Q}_1$, (7″)

follows simply

$$s_{21} = -s_{11}$$

and

$$\mathbf{Q}_3 = \mathbf{Q}_1(s_{21} = -s_{11}) = \begin{bmatrix} s_{11} & s_{11} & 0 \\ -s_{11} & s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}. \qquad (10c)$$

The possibility of **S** having the two non-equivalent forms $\mathbf{Q}_2$ and $\mathbf{Q}_3$ only exists for the groups $P422$, $P4mm$, $P4/mmm$, $P4_122$, $P4_322$, $P4_222$, $P4cc$, $P4/mcc$, $I422$, $I4mm$, $I4/mmm$. There are two remarkable exceptions: $P4/nmm$ only allows $\mathbf{Q}_2$ because the n glide is compatible only with the parallel orientation of the m planes in G and g. The case of $I4_122$ which allows only $\mathbf{Q}_2$ will be discussed later.

When the last two elements of the HM symbols are not identical, the parallel orientation alone is allowed and only the diagonal form $\mathbf{Q}_2$ is possible. However, $\mathbf{Q}_3$ is able to relate non-equivalent space groups which are 'class equivalent' (see Appendix B).

3.1.2. *Hexagonal and trigonal.* Here,

$$\alpha = \mathbf{6} = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \qquad (13)$$

Its commutation with **S** leads to the following general form of **S** in the hexagonal system;

$$\mathbf{H}_1 = \begin{bmatrix} s_{11} & s_{22} - s_{11} & 0 \\ s_{11} - s_{22} & s_{22} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}, \qquad (14a)$$

with

$$\det \mathbf{H}_1 = s_{33}(s_{11}^2 + s_{22}^2 - s_{11}s_{22}). \qquad (15)$$

This remains the only form of **S** for the classes 6, $\bar{6}$ and $6/m$ but also for the trigonal groups and rhombohedral groups (hexagonal axes) belonging to the classes 3 and $\bar{3}$, because from the commutation of **S** with $\alpha = \mathbf{6}$ also follows the commutation with $(\alpha)^2 = \mathbf{3}$.

When in the hexagonal space group symbol, the last two (binary) symmetry elements are different, their orientation in G and in g must be the same and their commutation with **S** implies

$$s_{22} = s_{11}$$

and

$$\mathbf{H}_2 = \mathbf{H}_1(s_{22} = s_{11}) = \begin{bmatrix} s_{11} & 0 & 0 \\ 0 & s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}. \qquad (14b)$$

When the last two elements of the HM symbol are identical, other orientations are allowed. In 622 for instance, the 2_x axis in G (say α) may coincide with the twofold axis of the second kind in g. Thus

$$\beta = \begin{bmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}, \quad \alpha = \begin{bmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}. \qquad (16)$$

From (7),

$$\mathbf{H}_1\beta = \alpha\mathbf{H}_1, \qquad (7'')$$

it follows by identification of the coefficients that

$$s_{22} - s_{11} = s_{11},$$

so that finally one obtains a matrix $\mathbf{H}_3$,

$$\mathbf{H}_3 = \mathbf{H}_1(s_{22} = 2s_{11}) = \begin{bmatrix} s_{11} & s_{11} & 0 \\ -s_{11} & 2s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}. \qquad (14c)$$

The possibility of **S** having the two (non-equivalent) forms $\mathbf{H}_2$ and $\mathbf{H}_3$ only exists for the groups *P*622, *P*6*mm*, *P*6/*mmm*, $P6_122$, $P6_522$, $P6_222$, $P6_422$, $P6_322$, *P*6*cc*, *P*6/*mcc*. When the last two elements of the HM symbol are different, $\mathbf{H}_3$ is still able to relate non-equivalent groups which are 'class equivalent' (see Appendix B).

Remark

When referred to hexagonal axes, the rhombohedral groups belong to $\mathbf{H}_1$ for *R*3 and $R\bar{3}$ and to $\mathbf{H}_2$ for *R*32, *R*3*m*, $R\bar{3}m$, *R*3*c* and $R\bar{3}c$. When referred to rhombohedral axes, the corresponding matrices are $\mathbf{R}_1$ and $\mathbf{R}_2$, respectively.

$$\mathbf{R}_1 = \begin{bmatrix} s_1 & s_2 & s_3 \\ s_3 & s_1 & s_2 \\ s_2 & s_3 & s_1 \end{bmatrix}, \qquad (17a)$$

$$\mathbf{R}_2 = \mathbf{R}_1(s_2 = s_3) = \begin{bmatrix} s_1 & s_2 & s_2 \\ s_2 & s_1 & s_2 \\ s_2 & s_2 & s_1 \end{bmatrix}. \qquad (17b)$$

Their determinants are

$$\det \mathbf{R}_1 = (s_1 + s_2 + s_3) \times (s_1^2 + s_2^2 + s_3^2 - s_1 s_2 - s_2 s_3 - s_3 s_1), \qquad (18a)$$

$$\det \mathbf{R}_2 = (s_1 + 2s_2)(s_1 - s_2)^2. \qquad (18b)$$

3.1.3. *Monoclinic.* If we consider a monoclinic crystal with the preferred direction along *Oz* (first setting of *International Tables for X-ray Crystallography*, 1952), the commutation of **S** with the matrix $\mathbf{2}_z$ or $\mathbf{m}_z$ ($\mathbf{m}_z$ = mirror perpendicular to *Oz*) reduces **S** to the form

$$\mathbf{M} = \begin{bmatrix} s_{11} & s_{12} & 0 \\ s_{21} & s_{22} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}, \qquad (19)$$

with

$$\det \mathbf{M} = s_{33}(s_{11}s_{22} - s_{21}s_{12}). \qquad (20)$$

The general matrices $\mathbf{Q}_1$ and $\mathbf{H}_1$ of the tetragonal and hexagonal systems are special cases of **M**. (The matrix **M** for the case '*b* axis unique' has non-diagonal terms s_{13} and s_{31}.)

$$\mathbf{Q}_1 = \mathbf{M}(s_{11} = s_{22}; s_{12} = -s_{21}), \qquad (21)$$

$$\mathbf{H}_1 = \mathbf{M}(s_{12} = -s_{21} = s_{22} - s_{11}). \qquad (22)$$

3.2. *Cubic and orthorhombic groups*

3.2.1. *Cubic.* The commutation rule leads to the 'spherical' matrix

$$\mathbf{C} = \begin{bmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{bmatrix}. \qquad (23)$$

It can be considered as special case of **M** (19) with $s_{11} = s_{22} = s_{33} = s$ and $s_{12} = s_{21} = 0$, or of $\mathbf{R}_1$ with $s_1 = s$ and $s_2 = s_3 = 0$.

For all cubic space groups the lowest index of a maximal equivalent subgroup is [27] (**a** = 3**A**, **b** = 3**B**, **c** = 3**C**) with the choice of origin as specified in *International Tables for X-ray Crystallography* (1952). For example, $P4_332$ is an equivalent subgroup of index [27] of $P4_132$. The isosymbolic maximal subgroup, say $P4_132$ has the index [125] (**a** = 5**A**, **b** = 5**B**, **c** = 5**C**) (*cf.* under § 4.1).

For all symmorphic cubic groups (*P*23, *F*23, *I*23, *etc.*) there exists an equivalent subgroup of index [8] (**a** = 2**A**, **b** = 2**B**, **c** = 2**C**) which however is *not* maximal. Indeed, consider a *P* lattice and double all lattice dimensions; the new unit cell contains eight points and the new lattice can be decomposed into either two *F* lattices or four *I* lattices.

Decentring gives rise to *P* lattices having an eight times larger unit cell. Chains of subgroups can be constructed as indicated below.

$$P \xrightarrow{[2]} F \xrightarrow{[4]} P \xrightarrow{[2]} F \cdots$$

or

$$P \xrightarrow{[4]} I \xrightarrow{[2]} P \xrightarrow{[4]} I \cdots$$

These chains also explain why *F* and *I* lattices have *non*-maximal equivalent subgroups of index [8].

3.2.2. *Orthorhombic.* When the three symmetry elements in the HM symbol are equivalent, there are six possible matrices, **S**, which correspond to the identical orientation ($\mathbf{O}_1$), to the circular permutation of the axes ($\mathbf{O}_2$ and $\mathbf{O}_3$) and to the interchange of two axes ($\mathbf{O}_4$,$\mathbf{O}_5$,$\mathbf{O}_6$).

$$\mathbf{O}_1=\begin{bmatrix} s_{11} & 0 & 0 \\ 0 & s_{22} & 0 \\ 0 & 0 & s_{33}\end{bmatrix};\quad \mathbf{O}_2=\begin{bmatrix} 0 & s_{12} & 0 \\ 0 & 0 & s_{23} \\ s_{31} & 0 & 0\end{bmatrix};$$

$$\mathbf{O}_3=\begin{bmatrix} 0 & 0 & s_{13} \\ s_{21} & 0 & 0 \\ 0 & s_{32} & 0\end{bmatrix};\quad \mathbf{O}_4=\begin{bmatrix} s_{11} & 0 & 0 \\ 0 & 0 & s_{23} \\ 0 & s_{32} & 0\end{bmatrix};\quad (24)$$

$$\mathbf{O}_5=\begin{bmatrix} 0 & 0 & s_{13} \\ 0 & s_{22} & 0 \\ s_{31} & 0 & 0\end{bmatrix};\quad \mathbf{O}_6=\begin{bmatrix} 0 & s_{12} & 0 \\ s_{21} & 0 & 0 \\ 0 & 0 & s_{33}\end{bmatrix}.$$

This is the case for *P*222, *Pmmm*, *Pnnn*, *F*222, *I*222, *Fmmm*, *Immm* and *Fddd*, and also for *C*222 and *Cmmm*, admitting here the equivalent of *A* and *B* centring.

One has the following rule: if one replaces the non-zero coefficients of the matrix $\mathbf{O}_j$ by 1 and if the corresponding transformation of the axes conserves the HM symbol, then $\mathbf{O}_j$ is allowed. For instance the circular permutation $x \to y \to z \to x$ leaves *Pbca* invariant. Indeed, $b_x \to c_y, c_y \to a_z, a_z \to b_x$. The same is true for the circular inverse permutation so that the matrices $\mathbf{O}_2$, $\mathbf{O}_3$ and $\mathbf{O}_1$ are allowed. A simple interchange of axes $x \leftrightarrows y$ changes *Pbca* to *Pcab* ($b_x \to a_y$, $c_y \to c_x$, $a_z \to b_z$) so that $\mathbf{O}_6$ is not allowed. Thus *we do not consider* here *different settings when they correspond to different HM symbols.** For *Ibca*, which has the full symbol I^{bca}_{cab}, all the matrices $\mathbf{O}_1$ to $\mathbf{O}_6$ are allowed; they leave the full symbol invariant.

When an axis or plane plays a privileged role, it generally corresponds to the *Oz* direction in the standard symbol of *International Tables for X-ray Crystallography* (1952). Two cases may occur:

(*a*) The symmetry operations corresponding to the *x* and *y* axes are equivalent and may be interchanged. Then the matrices $\mathbf{O}_1$ and $\mathbf{O}_6$ are allowed. This is the case for $P222_1$, $C222_1$, $P2_12_12$, *Pmm*2 and its *A*, *C*, *I* and *F* centring, *Pba*2, *Iba*2, *Pcc*2, *Ccc*2, *Pnn*2, *Fdd*2, *Pbam*, *Ibam*, *Pccm*, *Cccm*, *Pmmn*, *Pnnm*, *Pccn*, *Cmma*, *Imma*, *Ccca*.

(*b*) The symmetry operations corresponding to the *x* and *y* axes are not equivalent. Only the matrix $\mathbf{O}_1$ remains allowed. This is evident for *Pma*2 for instance. For *Pmma* and *Pnna* the non-equivalence of the *x* and *y* directions can be recognized from the full symbols which are respectively $P2_1/m\ 2/m\ 2/a$ and $P2/n\ 2_1/n\ 2/a$. In the interchange of *x* and *y*, the symbols would become *Pmmb* and *Pnnb* respectively. Consequently $\mathbf{O}_6$ is not allowed.

The triclinic groups *P*1 and $P\bar{1}$ are briefly considered in § 5.

* This does not imply any loss of generality (see Appendix C).

4. Parity rules

We now turn our attention to the relations (8*e*) and (8*b*), which in the presence of fractional lattice translations imposes 'parity'* conditions upon the coefficients of **S**. This will be the case for screw axes, glide planes (8*e*) and centred lattices (8*b*).

4.1. *Screw axes*

Suppose that the principal axis is a screw axis n_m and that the origin in *G* is on that axis. Relation (8*e*) can be written

$$s_{33}m/n - m/n = n_{33}\ \text{(integer)},$$

or

$$s_{33} = nn_{33}/m + 1. \qquad (25)$$

Thus, nn_{33}/m must be an integer (Buerger, 1947). We consider as an example $P4_1$. Here relation (25) becomes

$$s_{33} = 4n_{33} + 1$$

and the index of *g* is

$$\det \mathbf{Q}_1 = (4n_{33} + 1)(s_{11}^2 + s_{21}^2). \qquad (26)$$

Remark

Suppose that we increase the cell dimension only along **c**, keeping $s_{11}^2 + s_{21}^2 = 1$; then, for $n_{33} = 1, 2, 3$, we have isosymbolic subgroups $P4_1$ of index 5, 9, 13 respectively. For the negative values $n_{33} = -1, -2, -3$, one has $\det \mathbf{Q}_1 = -3, -7, -11$ respectively. The negative sign corresponds to a change of handedness, *i.e.* there are enantiomorphic subgroups $P4_3$ of index 3, 7 and 11 respectively of $P4_1$. At the same time we can answer the question of *maximal equivalent* subgroups. The subgroups of index 3, 5, 7, 11 and 13 are certainly maximal as these are prime numbers. The isosymbolic subgroup $P4_1$ of index nine is *not* maximal for we have the chain relation

$$P4_1 \to [3]\ P4_3 \to [3]\ P4_1.$$

If we had started with $P4_3$ we would have obtained the same result because 4_3 is identical to 4_1 provided the rotation is clockwise. We can also say, considering only moduli, *i.e.* positive numbers, that

$$s_{33} = 4n_{33} + 1$$

corresponds to subgroup relations

$$4_1 \to 4_1;\ 4_3 \to 4_3\ \text{(index 5, 9, 13 } \cdots\text{)}, \qquad (25a)$$

whilst

$$s_{33} = 4n_{33} + 3$$

corresponds to

$$4_1 \to 4_3;\ 4_3 \to 4_1\ \text{(index 3, 7, 11 } \cdots\text{)}. \qquad (25b)$$

* Exactly 'congruence modulo $\mathbb{Z}$'.

Similar considerations are valid for other enantiomorphic pairs such as $3_1, 3_2$; $6_1, 6_5$; $6_2, 6_4$.

There is no restriction on s_{11} and s_{21} so that the factor $s_{11}^2 + s_{21}^2$ takes the values 1, 2, 4, 5, 8, 9, 10, 13. If $n_{33} = 0$ for instance, those subgroups of index 2, 5, 13 are certainly maximal. It turns out that those of index 9 are also maximal; those of index 4, 8 and 10 are not (see Sayari, 1976 and Appendix D).

4.2. *Glide planes*

4.2.1. *Glide plane perpendicular to a principal axis.* Consider a glide plane operation n, $n = (m_z|\frac{1}{2}\frac{1}{2}0)$.

The relation (8*e*) for $\tau_\alpha = \frac{1}{2}\frac{1}{2}0$ becomes in a tetragonal lattice (matrix $\mathbf{Q}_1$)

$$(s_{11} \pm s_{21})/2 - \tfrac{1}{2} = p,$$

or

$$s_{11} \pm s_{21} = 2p + 1. \qquad (27)$$

Thus s_{11} and s_{21} must be of opposite parities. In $P4/n$ for instance, $s_{11}^2 + s_{21}^2$ can only take odd values 1, 5, 9, 13, *etc*. These opposite parities exclude for P_4/nmm the possibility of the matrix $\mathbf{Q}_3$ (where $s_{21} = s_{11}$).

4.2.2. *Glide plane parallel to a principal axis.* Consider the c operation as in $R3c$ for instance which sends point x, y, z to $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (in rhombohedral coordinates). Here τ_c is $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and relation (8*e*) leads to

$$(s_1 + 2s_2 - 1)/2 = n,$$

or

$$s_1 = 2n + 1. \qquad (29)$$

It is easily seen from det $\mathbf{R}_2$ that its minimum value occurs for $s_1 = -1$ and $s_2 = +1$ so that the maximal equivalent subgroup of $R3c$ has its lowest index equal to 4 and lattice vectors

$$\begin{aligned} \mathbf{a} &= -\mathbf{A} + \mathbf{B} + \mathbf{C}, \\ \mathbf{b} &= -\mathbf{B} + \mathbf{C} + \mathbf{A}, \\ \mathbf{c} &= -\mathbf{C} + \mathbf{A} + \mathbf{B}. \end{aligned} \qquad (30)$$

4.3. *Centred lattices*

As an application of (8*b*) we consider an I lattice in a tetragonal space group which for $\mathbf{S} = \mathbf{Q}_1$ introduces the following relations:

$$\begin{bmatrix} (s_{11} - s_{21})/2 \\ (s_{11} + s_{21})/2 \\ s_{33}/2 \end{bmatrix} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} n_1 + \frac{1}{2} \\ n_2 + \frac{1}{2} \\ n_3 + \frac{1}{2} \end{bmatrix}. \qquad (28)$$

Either s_{11} and s_{21} are of the same parity and s_{33} is even or s_{11} and s_{21} are of opposite parity and s_{33} is odd. In $I4$ one has both possibilities whilst in $I4_1$ only the latter can exist. Indeed, 4_1 *and* 4_3 axes are present here, so that s_{33} can take the values of (25*a*) *and* (25*b*), *i.e.* $s_{33} = 2n + 1$. The opposite parities of s_{11} and s_{21} in $I4_1$ also exclude the possibility of the matrix $\mathbf{Q}_3$ for $I4_122$ (whilst $\mathbf{Q}_3$ is allowed for $P4_122$).

Furthermore, if we associate with $I4_1$ a symmetry element such as m_x to form $I4_1md$ (so that only $\mathbf{Q}_2$ is allowed where $s_{21} = 0$, say *even*), then s_{11} can only be odd.

4.4. *Influence of the choice of origin*

To illustrate the influence of the choice of the origin on the parity of s_{ij} we shall discuss more thoroughly two examples $I4_1/a$ and $P2_12_12_1$.

4.4.1. *Discussion of* $I4_1/a$. There are two versions given in *International Tables for X-ray Crystallography* (1952) concerning the choice of the origin. We shall add a third one.

(1) *The origin is on the* $\bar{4}$ *axis.* We shall consider as generators the lattice translations of I (000; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$), and the operations of $(\bar{4}|000)$ and $(\bar{1}|0\frac{1}{2}\frac{1}{4})$ located at $0,0,z$ and $0,\frac{1}{4},\frac{1}{8}$, respectively. There are two solutions for the coordinate triplets X_o, Y_o, Z_o of the origin in g, labelled (*a*) and (*b*) and given in example 3 of Appendix A according to the two possible choices for t_G (integral and fractional translations). The matrix $\mathbf{S}$ has the form $\mathbf{Q}_1$ and the equation (8*a*) applied to the inversion operator $i = (\bar{1}|0\frac{1}{2}\frac{1}{4})$ reads

$$\begin{bmatrix} -s_{21}/2 \\ (s_{11} - 1)/2 \\ (s_{33} - 1)/4 \end{bmatrix} + 2\begin{bmatrix} X_o \\ Y_o \\ Z_o \end{bmatrix} = t_G. \qquad (31)$$

Here again we have two choices for t_G which we shall call α and β for integral and fractional translations respectively. For the four possibilities: $a\alpha$, $a\beta$, $b\alpha$ and $b\beta$ one finds the following parities of the coefficients s_{ij} (Table 1).

We recall that (*a*) corresponds to the choice 000 (and equivalents) whilst (*b*) corresponds to $0,\frac{1}{2},\frac{1}{4}$ (and equivalents) for the origins in g. Sets (*a*) and (*b*) are the locations of the centres of equivalent $\bar{4}$ axes.

(2) *The origin is at the inversion centre.* The following generators will be chosen: $i = (\bar{1}|000)$; $4_1 =$

Table 1. *Parity conditions*

Origin o on $\bar{4}$, group $I4_1/a$.

	$a\alpha$	$a\beta$	$b\alpha$	$b\beta$
s_{11}	$2p+1$	$2p$	$2p+1$	$2p$
s_{21}	$2q$	$2q+1$	$2q$	$2q+1$
s_{33}	$4r+1$	$4r-1$	$4r+1$	$4r+1$

o is at 000; $00\frac{1}{2}$; $\frac{1}{2}\frac{1}{2}0$; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ for the columns under $a\alpha$ and $a\beta$
at $\frac{1}{2}0\frac{1}{4}$; $\frac{1}{2}0\frac{3}{4}$; $0\frac{1}{2}\frac{1}{4}$; $0\frac{1}{2}\frac{3}{4}$ for the columns under $b\alpha$ and $b\beta$.

Origin o on 4_1

o is as above for the columns under $a\alpha$ and $b\alpha$
o is at $\frac{1}{2}00$; $\frac{1}{2}0\frac{1}{2}$; $0\frac{1}{2}0$; $0\frac{1}{2}\frac{1}{2}$ for the column under $a\beta$
o is at $00\frac{1}{4}$; $00\frac{3}{4}$; $\frac{1}{2}\frac{1}{2}\frac{1}{4}$; $\frac{1}{2}\frac{1}{2}\frac{3}{4}$ for the last column.

$(4_z|\frac{3}{4}\frac{1}{4}\frac{1}{4})$ and the translations 000; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ of I. The coordinates X_o, Y_o, Z_o can take the values 0 and/or $\frac{1}{2}$ (solution *a*) and $\pm\frac{1}{4}$ (solution *b*) according to example 1 of Appendix A.

Relation (8*a*) written for the symmetry element 4_1 becomes

$$\begin{bmatrix}(3s_{11}-s_{21}-3)/4\\(3s_{21}+s_{11}-1)/4\\(s_{33}-1)/4\end{bmatrix}+\begin{bmatrix}X_o+Y_o\\-X_o+Y_o\\0\end{bmatrix}=t_G. \quad (32)$$

The possible values of $X_o+Y_o=X'_o$ and $-X_o+Y_o=Y'_o$ are 00, $\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0$ and $0\frac{1}{2}$. Table 2 reproduces the result of the discussion.

It is remarkable that with the choice (*a*) of possible origins (in 000 for instance), s_{11} is always odd whilst for choice (*b*) (in $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ for instance), s_{11} is always even. Note again that the sets (*a*) and (*b*) are inversion centres.

(3) *Origin at* 4_1. We consider the generators $4_1=(4_z|00\frac{1}{4})$; $i=(\bar{1}|\frac{1}{2}0\frac{1}{4})$. The respective symmetry elements are located at $00z$ and $\frac{1}{4}0\frac{1}{8}$. Equation (8*a*) becomes explicitly

$$\begin{bmatrix}(s_{11}-1)/2\\s_{21}/2\\(s_{33}-1)/4\end{bmatrix}+2\begin{bmatrix}X_o\\Y_o\\Z_o\end{bmatrix}=t_{1G} \quad (33)$$

when written for i, and

$$\begin{bmatrix}0\\0\\(s_{33}-1)/4\end{bmatrix}+\begin{bmatrix}X_o+Y_o\\-X_o+Y_o\\+0\end{bmatrix}=t_{2G} \quad (34)$$

when written for 4_1.

If we split (8*a*) into the two equations (8*d*), we find as possible origins those given in the example 1 of Appendix A under (*a*) (point 000 and equivalents) and under (*b*) (point $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ and equivalents) with the solutions

$$s_{11}=2p+1;\quad s_{21}=2q;\quad s_{33}=4r+1 \text{ for } (a), \quad (35)$$

$$s_{11}=2p;\quad s_{21}=2q+1;\quad s_{33}=4r-1 \text{ for } (b). \quad (36)$$

It is then easily seen that the choice (*b*) of origins in g is not compatible with (34). The question arises if the set (*a*) of origins is complete. The answer is no. We still have to investigate the possibility of Z_o taking the value $\frac{1}{4}$. It then turns out that $\frac{1}{2}0\frac{1}{4}$ and $0\frac{1}{2}\frac{1}{4}$ are compatible with the parity conditions

$$s_{11}=2p+1;\quad s_{21}=2q;\quad s_{33}=4r-1, \quad (37)$$

(for t_{1G} integral and t_{2G} fractional) whilst the origins $00\frac{1}{4}$ and $\frac{1}{2}\frac{1}{2}\frac{1}{4}$ are compatible with the parity conditions

$$s_{11}=2p;\quad s_{21}=2q+1;\quad s_{33}=4r+1 \quad (38)$$

(for t_{1G} fractional and t_{2G} integral). Note again that the only origins possible in g are on 4_1 axes here, but that the parity conditions (35) to (38) are still the same as in Table 1.

To summarize the discussion, once the origin is chosen in G on a symmetry element, the origin in g is on a symmetry element of the same nature [see discussion following (8*c*)]. Parity conditions on the coefficients of **S** depend on the origin.

4.4.2 *Discussion of* $P2_12_12_1$. As a second example we discuss $P2_12_12_1$, the **S** matrix being $\mathbf{O}_6$. The generators $2_{1x}=(2_x|\frac{1}{2}\frac{1}{2}0)$ and $2_{1y}=(2_y|0\frac{1}{2}\frac{1}{2})$ as well as their product $2_{1z}=(2_z|\frac{1}{2}0\frac{1}{2})$ have the same form in G and in g. However the x and y axes are interchanged. For instance (8*a*) reads

$$\mathbf{O}_6\,\tau(2_{1x})-\tau(2_{1y})+[(\mathbf{1})-2_y]\mathbf{T}=t_G \quad (39)$$

and gives rise to the three equations

$$\begin{aligned}s_{12}/2+0+2X_o&=n_1,\\ s_{21}/2-\tfrac{1}{2}+0&=n_2,\\ 0-\tfrac{1}{2}+2Z_o&=n_3.\end{aligned} \quad (40)$$

Similar equations written for 2_{1y} and 2_{1z} give rise to the result that the coefficients of $\mathbf{O}_6$ must be odd, the origin being at $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ in g.

Thus one has finally 16 possible origins in $P2_12_12_1$ for o which are: 000; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ (for the matrices $\mathbf{O}_1$, $\mathbf{O}_2$, $\mathbf{O}_3$); $\frac{1}{4}\frac{1}{4}\frac{1}{4}$; $\frac{3}{4}\frac{3}{4}\frac{3}{4}$ (for the matrices $\mathbf{O}_4$, $\mathbf{O}_5$, $\mathbf{O}_6$) and those obtained by adding the translations 000, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}0\frac{1}{2}$ and $0\frac{1}{2}\frac{1}{2}$. Note that these remarkable points are not given explicitly in *International Tables for X-ray Crystallography* (1952) and that they are not located at symmetry elements.

Table 2. *Parity conditions*

Origin at the inversion centre, group $I4_1/a$

X_o, Y_o	00; $\frac{1}{2}\frac{1}{2}$		$0\frac{1}{2}$; $\frac{1}{2}0$		$\frac{1}{4}\frac{1}{4}$; $\frac{3}{4}\frac{3}{4}$		$\frac{1}{4}\frac{3}{4}$; $\frac{3}{4}\frac{1}{4}$	
X'_o, Y'_o	00		$\frac{1}{2}\frac{1}{2}$		$\frac{1}{2}0$		$0\frac{1}{2}$	
$s_{33}=4r+1$								
s_{11}	$4p+1$	$4p-1$	$4p+1$	$4p-1$	$4p$	$4p+2$	$4p$	$4p+2$
s_{21}	$4q$	$4q+2$	$4q+2$	$4q$	$4q-1$	$4q+1$	$4q+1$	$4q-1$
$s_{33}=4r-1$								
s_{11}	$4p+1$	$4p-1$	$4p+1$	$4p-1$	$4p$	$4p+2$	$4p$	$4p+2$
s_{21}	$4q+2$	$4q$	$4q$	$4q+2$	$4q+1$	$4q-1$	$4q-1$	$4q-1$

5. Equivalent subgroups of $P1$ and $P\bar{1}$

$P1$ occupies a special place as it has solely equivalent subgroups. Its discussion will be given in a separate paper (Billiet & Le Coz, 1979) and only the main results for subgroups g of prime index p will be reproduced here with

$$\mathbf{a} = p\mathbf{A};\quad \mathbf{b} = \mathbf{B} + q_1\mathbf{A};\quad \mathbf{c} = \mathbf{C} + q_2\mathbf{A} \quad (41)$$

and similar formulae obtained by circular permutation (as $\mathbf{b} = p\mathbf{B}$ and so on). q_1 and q_2 obey the important constraint

$$-\tfrac{1}{2}p < q_j \le \tfrac{1}{2}p. \quad (42)$$

For instance, $2\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ is a cell obtained by doubling one cell dimension ($p = 2$; $q_1 = q_2 = 0$).

$2\mathbf{A}$, $\mathbf{B} + \mathbf{A}$, $\mathbf{C}$, say the cell $p = 2$; $q_1 = 1$; $q_2 = 0$ is related to C centring. Indeed, subtracting $\mathbf{B} + \mathbf{A}$ from $2\mathbf{A}$ one does not change the cell volume and obtains $\mathbf{A} - \mathbf{B}$, $\mathbf{A} + \mathbf{B}$, $\mathbf{C}$.

$2\mathbf{A}$, $\mathbf{B} + \mathbf{A}$, $\mathbf{C} + \mathbf{A}$, say the cell $\mathbf{p} = 2$, $q_1 = q_2 = 1$ is related to face centring. Indeed, subtracting from $2\mathbf{A}$ the vectors $\mathbf{B} + \mathbf{A}$ and $\mathbf{C} + \mathbf{A}$ gives rise to the cell $-\mathbf{B} - \mathbf{C}$, $\mathbf{B} + \mathbf{A}$, $\mathbf{C} + \mathbf{A}$ or, changing the order of axes and conserving the handedness to $\mathbf{B} + \mathbf{C}$, $\mathbf{C} + \mathbf{A}$, $\mathbf{A} + \mathbf{B}$ which is the classical P lattice corresponding to face centring. The corresponding $\mathbf{S}$ matrix (1) is

$$\mathbf{S} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}. \quad (43)$$

The treatment of $P\bar{1}$ is analogous to that of $P1$. For monoclinic space groups (unique axis c) and two-dimensional groups $p1$ and $p\bar{1}$ one still has (41) and (42), dropping the parts related to $\mathbf{c}$.

6. Subgroups and supergroups

If g is a subgroup of G, conversely G is a supergroup for the group g. Thus equivalent supergroups are obtained by the inversion of (1) and (C'), say

$$(\mathbf{A},\mathbf{B},\mathbf{C}) = (\mathbf{a},\mathbf{b},\mathbf{c})\mathbf{S}^{-1}, \quad (1')$$

$$\mathsf{a} = \mathsf{S}\mathsf{b}\mathsf{S}^{-1}.$$

As an example of the application of (1′), we consider the relation just discussed in $P1$,

$$\mathbf{a}, \mathbf{b}, \mathbf{c} = \mathbf{B} + \mathbf{C}, \mathbf{C} + \mathbf{A}, \mathbf{A} + \mathbf{B}, \quad (44)$$

between the unit-cell vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the (face centred) P lattice of g and $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ of the group G. We can ask the inverse question: if $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are the lattice vectors of the group g, what are the lattice vectors $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ of the supergroup G? One reads at once from (44) that

$$\tfrac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c}) = \mathbf{A} + \mathbf{B} + \mathbf{C}, \quad (45)$$

so that the lattice of the supergroup G is I centred.

By elementary calculations one has [subtracting (44) from (45)]

$$\mathbf{A} = \tfrac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c});\quad \mathbf{B} = \tfrac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c});$$
$$\mathbf{C} = \tfrac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c}), \quad (46)$$

and one checks at once that the matrix $\mathbf{S}'$ (47) is the inverse of the matrix $\mathbf{S}$ (47) and that $\det \mathbf{S}' = \tfrac{1}{2}$,

$$\mathbf{S}' = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{bmatrix} = \mathbf{S}^{-1}. \quad (47)$$

To show once more the reversibility of the group–subgroup relations, we consider the transformation (48) which corresponds to $s_{11} = s_{22} = s_{33} = 1$ in the matrix $\mathbf{H}_3$ (14c);

$$\mathbf{a} = \mathbf{A} - \mathbf{B},\quad \mathbf{b} = \mathbf{A} + 2\mathbf{B},\quad \mathbf{c} = \mathbf{C}. \quad (48)$$

The resolution with respect to $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ is given by (49) where now the vectors $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ define the cell dimensions of the lattice of the *supergroup* G, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ being those of the *group* g;

$$\mathbf{A} = \tfrac{1}{3}(2\mathbf{a} + \mathbf{b}),\quad \mathbf{B} = \tfrac{1}{3}(-\mathbf{a} + \mathbf{b}),\quad \mathbf{C} = \mathbf{c}. \quad (49)$$

The matrix formed by the coefficients of (49) is of course the inverse of that of (48), the general solution being

$$(\mathbf{H}_3)^{-1} = \begin{bmatrix} 2/3s_{11} & -1/3s_{11} & 0 \\ 1/3s_{11} & 1/3s_{11} & 0 \\ 0 & 0 & 1/3s_{33} \end{bmatrix}. \quad (50)$$

Thus, considering subgroups *and* supergroups, the similarity operators S which relate equivalent groups G and g form themselves an infinite group, the existence of the element identity $\mathsf{S}_0 = (1|000)$, of the inverse and of a multiplication rule being easily proven.

For this last point, consider the group G, a subgroup g of G and a subgroup h of g. Let $\mathsf{a} = (\alpha|\tau_\alpha)$, $\mathsf{b} = (\beta|\tau^\beta)$, $\mathsf{c} = (\gamma|\tau_\gamma)$ be homologous symmetry operators in G, g and h respectively. One has the conjugation relations

$$\mathsf{a}\mathsf{S}_1 = \mathsf{S}_1\mathsf{b} \quad \text{and} \quad \mathsf{b}\mathsf{S}_2 = \mathsf{S}_2\mathsf{c}, \quad (51)$$

from which follows the existence of a multiplication law

$$\mathsf{a}\mathsf{S}_1\mathsf{S}_2 = \mathsf{S}_1\mathsf{S}_2\mathsf{c}. \quad (52)$$

7. Tabulation of maximal equivalent subgroups of lowest index

Tables 3 to 6 indicate the space groups, preceded by their number as in *International Tables for X-ray Crystallography* (1952), the lowest index of the equivalent subgroup for different axes and the cor-

Table 3. *Monoclinic*

	A	B	C	Conditions
Unique axis *C*				
$3P2$; $6Pm$; $10P2/m$.	[2]2**A**; [2]2**A**, **B** − **A**.	[2]2**B**; [2]**A** − **B**, 2**B**.	[2]	
$4P2_1$; $11P2_1/m$.	[2]2**A**; [2]2**A**, **B** − **A**.	[2]2**B**; [2]**A** − **B**, 2**B**.	[3]	s_{33} odd.
$7Pb$; $13P2/b$.	[2]2**A**. –	[3]3**B**; [3]**A** ± **B**, 3**B**	[2]	s_{12} even, s_{22} odd.
$14P2_1/b$.	[2]2**A**. –	[3]3**B**; [3]**A** ± **B**, 3**B**.	[3]	s_{12} even, s_{22} and s_{33} odd.
$5B2$; $8Bm$; $12B2/m$.	[3]3**A**; [3]3**A**, **B** ± **A**.	[2]2**B**; –	[3]	$s_{11} + s_{22}$ even, s_{21} even.
$9Bb$; $15B2/b$.	[3]3**A**; [3]3**A**, **B** ± **A**.	[3]3**B**; [3]**A** ± 2**B**, 3**B**.	[3]	$s_{11} + s_{33}$ even, s_{21} even, s_{22} odd.
Other cell choices				
$7Pn$; $13P2/n$.	– [2]2**A**, **B** − **A**.	– [2]**A** − **B**, 2**B**.	[2]	$s_{11} + s_{12}$ and $s_{21} + s_{22}$ odd.
$14P2_1/n$.	– [2]2**A**, **B** − **A**.	– [2]**A** − **B**, 2**B**.	[3]	$s_{11} + s_{12}$, $s_{21} + s_{22}$ and s_{33} odd.
$5I2$; $8Im$; $12I2/m$.	– [2]2**A**, **B** − **A**.	– [2]**A** − **B**, 2**B**.	[3]	$s_{11} + s_{12}$, $s_{21} + s_{22}$ and s_{33} of same parity.
$9Ib$; $15I2/b$.	[3]3**A**; [3]3**A**, **B** ± 2**A**.	[3]3**B**; [3]**A** ± 2**B**, 3**B**.	[3]	$s_{11} + s_{12}$, $s_{21} + s_{22}$ and s_{33} of same parity; $s_{12} + s_{22}$ odd.

Only directions **A** and **B** are considered. The information given is redundant when these directions are equivalent. On the other hand the information is incomplete for the other cell choices (except 9 and 15) where the index [3] would be found for the direction **A** + **B**.

Table 4. *Orthorhombic*

	A		B		C	Conditions
$16P222$; $47Pmmm$.	[2]	or	[2]	or	[2]	
$21C222$; $25Pmm2$.	[2]	or	[2]		[2]	
$17P222_1$; $27Pcc2$; $49Pccm$.	[2]	or	[2]		[3]	s_{33} odd.
$26Pmc2_1$.	[2]		[2]		[3]	s_{33} odd.
$28Pma2$; $51Pmma$.	[3]		[2]		[2]	s_{11} odd.
$18P2_12_12$; $32Pba2$; $50Pban$; $55Pbam$; $59Pmmn$; $67Cmma$.	[3]	or	[3]		[2]	s_{11}, s_{22} odd.
$35Cmm2$; $65Cmmm$.						$s_{11} + s_{22}$ even.
$29Pca2_1$; $31Pmn2_1$; $53Pmna$; $54Pcca$.	[3]		[2]		[3]	s_{11}, s_{33} odd.
$30Pnc2$; $39Abm2$; $57Pbcm$.	[2]		[3]		[3]	s_{22}, s_{33} odd.
$38Amm2$.						$s_{22} + s_{33}$ even.
$19P2_12_12_1$; $24I2_12_12_1$; $48Pnnn$; $61Pbca$; $70Fddd$; $73Ibca$. *	[3]	or	[3]	or	[3]	s_{11}, s_{22}, s_{33} odd.
$22F222$; $23I222$; $69Fmmm$; $71Immm$.						s_{11}, s_{22}, s_{33} same parity.
$34Pmn2$; $43Fdd2$; $45Iba2$; $56Pccn$; $68Ccca$; $58Pnnm$; $72Ibam$; $74Imma$.	[3]	or	[3]		[3]	s_{11}, s_{22}, s_{33} odd.
$44Imm2$; $42Fmm2$.						s_{11}, s_{22}, s_{33} same parity.
$20C222_1$; $37Ccc2$; $66Cccm$.						s_{11}, s_{22} same parity; s_{33} odd.
$33Pna2_1$; $41Aba2$; $46Ima2$; $52Pnna$; $60Pbcn$; $62Pnma$; $64Cmca$.	[3]		[3]		[3]	s_{11}, s_{22}, s_{33} odd.
$36Cmc2_1$; $63Cmcm$.						$s_{11} + s_{22}$ even; s_{33} odd.
$40Ama2$.						s_{11} odd; $s_{22} + s_{33}$ even.

All conditions are given for the matrix $\mathbf{O}_1$.
'or' means 'equivalent'.

responding vector relations. The groups under consideration are monoclinic (Table 3), orthorhombic (Table 4), tetragonal (Table 5), trigonal, rhombohedral and hexagonal (Table 6). The last column of the tables indicates general parity conditions on the coefficients of the **S** matrix.

As an example, the line in Table 3 relative to the groups $B11b$ (No. 9) and $B112/b$ (No. 15) gives the following information. The lowest index of equivalent groups is [3]. The vector relations are:

$$\mathbf{a} = 3\mathbf{A},\quad \mathbf{b} = \mathbf{B},\quad \mathbf{c} = \mathbf{C};$$
$$\mathbf{a} = 3\mathbf{A},\quad \mathbf{b} = \mathbf{A} + \mathbf{B},\quad \mathbf{c} = \mathbf{C};$$
$$\mathbf{a} = 3\mathbf{A},\quad \mathbf{b} = -\mathbf{A} + \mathbf{B},\quad \mathbf{c} = \mathbf{C};$$
$$\mathbf{a} = \mathbf{A},\quad \mathbf{b} = 3\mathbf{B},\quad \mathbf{c} = \mathbf{C};$$
$$\mathbf{a} = \mathbf{A} + 2\mathbf{B},\quad \mathbf{b} = 3\mathbf{B},\quad \mathbf{c} = \mathbf{C};$$
$$\mathbf{a} = \mathbf{A} - 2\mathbf{B},\quad \mathbf{b} = 3\mathbf{B},\quad \mathbf{c} = \mathbf{C};$$
$$\mathbf{a} = \mathbf{A},\quad \mathbf{b} = \mathbf{B},\quad \mathbf{c} = 3\mathbf{C};$$

and the coefficients in

$$\mathbf{a} = s_{11}\mathbf{A} + s_{21}\mathbf{B},\ \mathbf{b} = s_{12}\mathbf{A} + s_{22}\mathbf{B},\ \mathbf{c} = s_{33}\mathbf{C}$$

are such, that s_{22} is odd (here 1 or 3), s_{21} is even (here 0 or ± 2) and $s_{11} + s_{33}$ is even (here $1 + 3$ or $3 + 1$).

The authors are indebted to Professor David Shoemaker for critical reading and valuable corrections.

Note added in proof: Recently, Koch & Fischer (1978) have given a definition of the 'affine isomorphism' which is related to our definition of the 'conjugation relation' (Bertaut & Billiet, 1978).

Table 5. *Tetragonal*

	C	A,B	Conditions
75 $P4$; 81 $P\bar{4}$; 83 $P4/m$; 89 $P422$; 99 $P4mm$; 123 $P4/mmm$.	[2]	[2]	
76 $P4_1$;* 78 $P4_3$;* 91 $P4_122$;* 95 $P4_322$;* 77 $P4_2$; 84 $P4_2/m$; 103 $P4cc$; 124 $P4/mcc$.	[3]	[2]	s_{33} odd.
85 $P4/n$.	[2]	[5]	$s_{11} + s_{21}$ odd ($\mathbf{Q}_1$).
79 $I4$; 82 $I\bar{4}$; 87 $I4/m$.	[3]	[5]	$s_{11} + s_{21}$ and s_{33} same parity ($\mathbf{Q}_1$).
80 $I4_1$; 86 $P4_2/n$; 88 $I4_1/a$.			$s_{11} + s_{21}$ and s_{33} odd.
90 $P42_12$; 100 $P4bm$; 113 $P\bar{4}2_1m$; 117 $P\bar{4}b2$; 125 $P4/n$; 127 $P4/mbm$; 129 $P4/nmm$.	[2]	[9]	s_{11} odd.
111 $P\bar{4}2m$;† 115 $P\bar{4}m2$.†			s_{11} arbitrary.
92 $P4_12_12$;* 94 $P4_22_12$; 96 $P4_32_12$;* 98 $I4_122$; 102 $P4_2nm$; 104 $P4nc$; 106 $P4_2bc$; 108 $I4cm$; 109 $I4_1md$; 110 $I4_1cd$; 114 $P\bar{4}2_1c$; 118 $P\bar{4}n2$; 120 $I\bar{4}c2$; 122 $I\bar{4}2d$; 126 $P4/nnc$; 128 $P4/mnc$; 130 $P4/ncc$; 133 $P4_2/nbc$; 134 $P4_2/nnm$; 135 $P4_2/mbc$; 136 $P4_2/mnm$; 137 $P4_2/nmc$; 138 $P4_2/ncm$; 140 $I4/mcm$; 141 $I4_1/amd$; 142 $I4_1/acd$.	[3]	[9]	s_{11} and s_{33} odd ($\mathbf{Q}_2$).
97 $I422$; 107 $I4mm$; 139 $I4/mmm$.			$s_{11} + s_{33}$ even ($\mathbf{Q}_2$) or s_{33} even ($\mathbf{Q}_3$).
119 $I\bar{4}m2$; 121 $I\bar{4}2m$.			$s_{11} + s_{33}$ even ($\mathbf{Q}_2$).
101 $P4_2cm$; 105 $P4_2mc$; 112 $P\bar{4}2c$; 116 $P\bar{4}c2$; 131 $P4_2/mmc$; 132 $P4_2/mcm$.			s_{33} odd.†

In the column **A**, **B** [2] abbreviates the transformation $\mathbf{a} = \mathbf{A} + \mathbf{B}$, $\mathbf{b} = -\mathbf{A} + \mathbf{B}$;
[5] abbreviates the transformation $\mathbf{a} = 2\mathbf{A} + \mathbf{B}$, $\mathbf{b} = -\mathbf{A} + 2\mathbf{B}$;
[9] abbreviates the transformation $\mathbf{a} = 3\mathbf{A}$, $\mathbf{b} = 3\mathbf{B}$.

* For the starred symbols the equivalent subgroup of index [3] has the symbol of the enantiomorphic group. The first isosymbolic maximal subgroup has the index [5] ($\mathbf{c} = 5\mathbf{C}$).

† The subgroup of index [4] $\mathbf{a} = 2\mathbf{A}$, $\mathbf{b} = 2\mathbf{B}$, $\mathbf{c} = 2\mathbf{C}$ is not maximal (*cf.* Appendix B).

Table 6. *Trigonal, rhombohedral, hexagonal*

	C	A,B
143 $P3$; 144 $P3_1$;* 145 $P3_2$;* 147 $P\bar{3}$; 168 $P6$; 171 $P6_2$;* 172 $P6_4$;* 174 $P\bar{6}$; 175 $P6/m$; 177 $P622$; 180 $P6_222$;* 181 $P6_422$;* 183 $P6mm$; 191 $P6/mmm$.	[2]	[3]
149 $P312$; 150 $P321$; 151 $P3_112$;* 152 $P3_121$;* 153 $P3_212$;* 154 $P3_221$;* 156 $P3m1$; 157 $P\bar{3}1m$; 162 $P31m$; 164 $P3m1$; 146 $R3$; 148 $R3$; 155 $R32$; 160 $R3m$; 166 $R3m$; 187 $P\bar{6}m2$; 189 $P\bar{6}2m$.	[2]	[4]
173 $P6_3$; 176 $P6_3/m$; 182 $P6_322$; 184 $P6cc$; 192 $P6/mcc$.	[3]	[3]
158 $P3c1$; 159 $P31c$; 163 $P\bar{3}1c$; 165 $P\bar{3}c1$; 185 $P6_3cm$; 186 $P6_3mc$; 188 $P\bar{6}c2$; 190 $P\bar{6}2c$; 193 $P6_3/mcm$; 194 $P6_3/mmc$.	[3]	[4]
169 $P6_1$; 170 $P6_5$; 178 $P6_122$; 179 $P6_522$.	[5]	[3]
161 $R3c$; 167 $R\bar{3}c$.	[5]	[4]

In the column **A**, **B**, [3] abbreviates the transformation $\mathbf{a} = \mathbf{A} - \mathbf{B}$, $\mathbf{b} = \mathbf{A} + 2\mathbf{B}$;
[4] abbreviates the transformation $\mathbf{a} = 2\mathbf{A}$, $\mathbf{b} = 2\mathbf{B}$.
For conditions see text §4.1. and §4.2.

* For the starred symbols, the equivalent subgroup of index [2] ($\mathbf{c} = 2\mathbf{C}$) has the symbol of the enantiomorphic group. The isosymbolic subgroup of index [4] ($\mathbf{c} = 4\mathbf{C}$) is not maximal. The first maximal isosymbolic subgroup has the index [7] ($\mathbf{c} = 7\mathbf{C}$).

APPENDIX A

Locations of equivalent symmetry elements and choice of origin

Examples:

(1) $$\alpha = \bar{1} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Equation (8*c*) reduces to

$$2(X_o,Y_o,Z_o) = t_G. \qquad (A1)$$

Thus in a *P* lattice the solutions are

(*a*) $X_o, Y_o, Z_o = 000; \frac{1}{2}00; 0\frac{1}{2}0; 00\frac{1}{2};$
$\frac{1}{2}\frac{1}{2}0; \frac{1}{2}0\frac{1}{2}; 0\frac{1}{2}\frac{1}{2}; \frac{1}{2}\frac{1}{2}\frac{1}{2}.$

In an *I* lattice, t_G can be a fractional translation which adds the following solutions;

(*b*) $X_o,Y_o,Z_o = \frac{1}{4}\frac{1}{4}\frac{1}{4}; \frac{1}{4}\frac{1}{4}\frac{3}{4}; \frac{3}{4}\frac{1}{4}\frac{1}{4}; \frac{1}{4}\frac{3}{4}\frac{1}{4};$
$\frac{3}{4}\frac{3}{4}\frac{1}{4}; \frac{1}{4}\frac{3}{4}\frac{3}{4}; \frac{3}{4}\frac{1}{4}\frac{3}{4}; \frac{3}{4}\frac{3}{4}\frac{3}{4}.$

The 16 coordinate triplets under (*a*) and (*b*) form the set of the locations of the symmetry centres in an *I* lattice.

(2) $$\alpha = 4 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Equation (8*c*) reduces to

$$(X_o + Y_o, -X_o + Y_o, 0) = t_G. \qquad (A2)$$

In a *P* lattice the solutions are

(*a*) $X_o, Y_o = 00; \frac{1}{2}\frac{1}{2}$ and Z_o arbitrary.

In an *I* lattice these solutions remain the same as under (*a*) because in (*A*2), fractional translations are not allowed for t_G. The situation is, however, different for a screw axis, say 4_1 (*cf.* § 4.4.1).

(3) $$\alpha = \bar{4} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Equation (8*c*) reduces to

$$(X_o - Y_o, X_o + Y_o, 2Z_o) = t_G. \qquad (A3)$$

In a *P* lattice the solutions are

(*a*) $X_o,Y_o,Z_o = 000; \frac{1}{2}\frac{1}{2}0; 00\frac{1}{2}; \frac{1}{2}\frac{1}{2}\frac{1}{2}.$

In an *I* lattice one has to add the positions

(*b*) $X_o,Y_o,Z_o = 0\frac{1}{2}\frac{1}{4}; 0\frac{1}{2}\frac{3}{4}; \frac{1}{2}0\frac{1}{4}; \frac{1}{2}0\frac{3}{4}.$

These eight coordinate triplets represent the centres of the $\bar{4}$ axes in an *I* lattice (example $I4_1/a$, space group No. 88, origin at $\bar{4}$).

(4) $$\alpha = 2_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

The solution is

$$(0,2Y_o,2Z_o) = t_G, \qquad (A4)$$

say,

$Y_o,Z_o = 00; \frac{1}{2}0; 0\frac{1}{2}; \frac{1}{2}\frac{1}{2}$ and X_o arbitrary

for a *P* lattice as well as an *I* lattice (fractional t_G are not allowed).

Thus, in $I\bar{4}$ there are eight possible **T** vectors, whilst in $I\bar{4}2m$ (generators $\bar{4}$ of example 3 and 2_x of example 4) only four are possible. In $I4/mmm$ (generators $\bar{1}$ of example 1, 4 of example 2, 2_x of example 4), the intersection of the solutions corresponding to the generators comprises the same four vectors: $000; \frac{1}{2}\frac{1}{2}0; 00\frac{1}{2}; \frac{1}{2}\frac{1}{2}\frac{1}{2}$.

(5) $$\alpha = 3 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

(rhombohedral or cubic axes).

The solution is

$$(X_o - Z_o, Y_o - X_o, Z_o - Y_o) = t_G. \qquad (A5)$$

Note that the sum of the coordinates on the left hand side is zero, so that t_G = fractional translation is not allowed in an *I* lattice (but is possible in an *F* lattice).

APPENDIX B

'Class-equivalent' space groups

If *G* is $P\bar{4}m2$, $g = P\bar{4}2m$ is a maximal subgroup of index 2. Although the space groups are different, their crystal classes are the same. That is why we call these space groups 'class equivalent'.

Provided we choose in Fig. 1 $\alpha_1 = m_X$, $\beta_1 = m_{xx}$ (or $\alpha_2 = 2_{XX}$, $\beta_2 = 2_y$) as homologous symmetry operators, relations (*C*) and more particularly (7) still hold with the result that $\mathbf{S} = \mathbf{Q}_3$. For $s_{11} = s_{33} = 1$, one finds

$$\mathbf{a}, \mathbf{b}, \mathbf{c} = \mathbf{A} - \mathbf{B}, \mathbf{A} + \mathbf{B}, \mathbf{C}. \qquad (B1)$$

The non-equivalence of *G* and *g* is also evident from the fact that det $\mathbf{Q}_3$ *cannot* take the value unity.

One may construct the infinite chain of subgroups:

$$P\bar{4}m2 \xrightarrow{[2]} P\bar{4}2m \xrightarrow{[2]} P\bar{4}m2 \longrightarrow \cdots.$$

Thus the equivalent subgroup $P\bar{4}m2$ of index 4 of $G = P\bar{4}m2$ is not maximal. Its unit-cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ are obtained by iteration of (*B*1). $\mathbf{a}', \mathbf{b}', \mathbf{c}' = \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c} = -2\mathbf{B}, 2\mathbf{A}, \mathbf{C}$ and correspond to doubling $\mathbf{A}$ and $\mathbf{B}$. Note that this result can also be obtained from $\mathbf{Q}_2$ with $s_{11}^{Q_2} = 2$.

More generally one has chains

$$P\bar{4}m2 \xrightarrow{[i]} P\bar{4}2m \xrightarrow{[i]} P\bar{4}m2 \longrightarrow \cdots,$$

where, assuming $s_{33}^{Q_2} = s_{33}^{Q_3} = 1$, the index $[i]$ is given by

$$[i] = 2(s_{11}^{Q_3})^2 \text{ and } s_{11}^{Q_2} = 2(s_{11}^{Q_3})^2. \qquad (B2)$$

Couples of class-equivalent space groups in the tetragonal system are:

($P4_2mc$ No. 105, $P4_2cm$ No. 101); ($P\bar{4}2m$ No. 111, $P\bar{4}m2$ No. 115); ($P\bar{4}2c$ No. 112, $P\bar{4}c2$ No. 116); ($I\bar{4}m2$ No. 119, $I\bar{4}2m$ No. 121); ($P4_2/mmc$ No. 131, $P4_2/mcm$ No. 132).

One similarly has 'class-equivalent space groups' of index 3 in trigonal and hexagonal space groups. Thus $G = P3m1$ and $g = P31m$ are related by the matrix $\mathbf{H}_3$ so that for $s_{11} = s_{33} = 1$ the vector relations between the unit cells are

$$\mathbf{a}, \mathbf{b}, \mathbf{c} = \mathbf{A} - \mathbf{B}, \mathbf{A} + 2\mathbf{B}, \mathbf{C}. \qquad (B3)$$

One may construct the infinite chain of subgroups

$$P3m1 \xrightarrow{[3]} P31m \xrightarrow{[3]} P3m1 \longrightarrow \cdots.$$

Thus the equivalent subgroup $P3m1$ of index 9 of $G = P3m1$ is not maximal. Its unit-cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ obtained by iteration of (*B*3) $\mathbf{a}', \mathbf{b}', \mathbf{c}' = \mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c} = -3\mathbf{B}, 3\mathbf{A} + 3\mathbf{B}, \mathbf{C}$ correspond to tripling the unit-cell vectors in G; this result may also be obtained from the matrix $\mathbf{H}_2$ with $s_{33}^{H_2} = 3$.

More generally one has chains

$$P3m1 \xrightarrow{[i]} P31m \xrightarrow{[i]} P3m1 \longrightarrow \cdots,$$

where, assuming $s_{33}^{H_2} = s_{33}^{H_3} = 1$, the index $[i]$ is given by

$$[i] = 3(s_{11}^{H_3})^2 \text{ and } s_{11}^{H_2} = 3(s_{11}^{H_3})^2. \qquad (B4)$$

Couples of class-equivalent space groups in the trigonal system are:

($P312$ No. 149, $P321$ No. 150); ($P3_112$ No. 151, $P3_121$ No. 152); ($P3_212$ No. 153, $P3_221$ No. 154); ($P3m1$ No. 156, $P31m$ No. 157); ($P3c1$ No. 158, $P31c$ No. 159); ($P\bar{3}1m$ No. 162, $P\bar{3}m1$ No. 164); ($P\bar{3}1c$ No. 163, $P\bar{3}c1$ No. 165)

and in the hexagonal system

($P6_3cm$ No. 185, $P6_3mc$ No. 186); ($P\bar{6}m2$ No. 187, $P\bar{6}2m$ No. 189); ($P\bar{6}c2$ No. 188, $P\bar{6}2c$ No. 190); ($P6_3/mcm$ No. 193, $P6_3/mmc$ No. 194).

Remark

Note that the matrix

$$\begin{bmatrix} s_{11} & -s_{11} & 0 \\ s_{11} & s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}$$

is equivalent to $\mathbf{Q}_3$.

Also the following matrices

$$\begin{bmatrix} 2s_{11} & -s_{11} & 0 \\ s_{11} & s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}, \begin{bmatrix} s_{11} & -2s_{11} & 0 \\ 2s_{11} & -s_{11} & 0 \\ 0 & 0 & s_{33} \end{bmatrix}$$

are equivalent to $\mathbf{H}_3$. By putting s_{11} and s_{33} equal to one the reader may check that he gets familiar axis transformations which are equivalent to (*B*1) and (*B*3) respectively.

APPENDIX C
On settings

The six 'setting' matrices $\mathbf{S}_j$ ($j = 1,\cdots, 6$) of the orthorhombic system which, according to (1) transform $\mathbf{a}, \mathbf{b}, \mathbf{c}$ to the settings $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{c}, \mathbf{a}, \mathbf{b}$; $\mathbf{b}, \mathbf{c}, \mathbf{a}$; $\mathbf{a}, \bar{\mathbf{c}}, \mathbf{b}$; $\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}$; $\bar{\mathbf{c}}, \mathbf{b}, \mathbf{a}$, in *International Tables for X-ray Crystallography* (1952) are:

$$\mathbf{S}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad \mathbf{S}_2 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix};$$
$$\mathbf{S}_3 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}; \quad \mathbf{S}_4 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix};$$
$$\mathbf{S}_5 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}; \quad \mathbf{S}_6 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}. \qquad (C1)$$

They belong to a group of 24 matrices of determinant +1, corresponding to all right-handed systems which may be constructed by permutations and/or changes of signs of the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$. This matrix group of similarity operators $\mathbf{S}_j$ ($j = 1, \cdots, 24$) is isomorphic to the point group 432-O. If one includes *all* settings, regardless of handedness, one has just to multiply the preceding 24 matrices by the inversion matrix

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

in order to obtain the complete group of all setting matrices which of course is isomorphic to the point group $m\bar{3}m$-O_h.

If the operators $a = (\alpha | \tau_\alpha)$ of G are expressed in the conventional setting and those of g, say $b = (\beta | \tau_\beta)$ in a non-conventional setting, belonging to a matrix $\mathbf{S}_j$, one has for the new operators $b' = (\beta' | \tau'_\beta)$,

$$b = (\mathbf{S}_j | 000)^{-1}\, b(\mathbf{S}_j | 000) = (\mathbf{SS}_j | \mathbf{T})^{-1}\, a(\mathbf{SS}_j | \mathbf{T}). \quad (C2)$$

One may consider more general changes of settings, $S = (\mathbf{S}_j | \mathbf{T}_j)$, involving a change of axes *and* of origin and use the general formula

$$b' = (SS_j)^{-1}\, a(SS_j). \quad (C3)$$

Example. If $\mathbf{S} = \mathbf{O}_1$ (24) and $\mathbf{S}_j = \mathbf{S}_5$ ($C1$), one has

$$\mathbf{SS}_j = \begin{bmatrix} 0 & s_{11} & 0 \\ s_{22} & 0 & 0 \\ 0 & 0 & -s_{33} \end{bmatrix}.$$

APPENDIX D
Factorization of matrices

Considering the 2×2 matrix part

$$\begin{bmatrix} s_{11} & -s_{21} \\ s_{21} & s_{11} \end{bmatrix}$$

of determinant $s_{11}^2 + s_{21}^2$, a subgroup is not maximal if the matrix can be factorized into matrices of the same nature (Sayari, 1976). For instance, the factorization scheme for the index $10 = 3^2 + 1^2$ is

$$\begin{bmatrix} 1 & -3 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix}, \quad (D1)$$

the intermediate subgroups having the indices $2 = 1^2 + 1^2$ and $5 = 2^2 + 1^2$.

References

BERTAUT, E. F. & BILLIET, Y. (1978). *C.R. Acad. Sci.* **287**, 989–991.
BILLIET, Y. (1973). *Bull. Soc. Fr. Minéral. Cristallogr.* **96**, 327–334.
BILLIET, Y. & LE COZ, M. (1979). *Acta Cryst.* To be submitted.
BUERGER, M. (1947). *J. Chem. Phys.* **15**, 1–16.
International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.
KOCH, E. & FISCHER, W. (1978). *Z. Kristallogr.* **147**, 21–38.
SAYARI, A. (1976). Thèse de spécialité, Tunis.

Acta Cryst. (1979). A**35**, 745–756

The Defect Structure of VO_x. I. The Ordered Phase, $VO_{1\cdot 30}$

BY M. MORINAGA* AND J. B. COHEN

Department of Materials Science & Engineering, The Technological Institute, Northwestern University, Evanston, IL 60201, USA

(*Received* 28 *November* 1978; *accepted* 13 *March* 1979)

Abstract

Integrated X-ray intensities were obtained from a single crystal of $VO_{1.30}$ annealed below the ordering transition. The space group is $I4_1/amd$, and the unit-cell contents are $V_{51.6}O_{64}$. The atomic arrangement is similar to that proposed by Andersson & Gjönnes [*Acta Chem. Scand.* (1970), **24**, 2250–2252], but there are more vanadium vacancies and interstitial ions. The latter are surrounded by four vacancies as in the defect structure of Fe_xO. The oxygen ions around an interstitial vanadium ion are displaced away from it; oxygen and vanadium ions on the octahedrally coordinated sites exhibit strongly correlated displacements. There are anisotropic electron density distributions at vanadium ions near a vacancy. These effects indicate that the order–disorder transition is not due to a Jahn–Teller effect, but instead is a result of a long-range cooperative interaction, presumably due to the semimetallic nature of this oxide.

* Now at Toyohashi University of Technology, Toyohashi, Aichi, 440, Japan.

0567-7394/79/050745-12$01.00

I. Introduction

VO_x contains large concentrations of cation and anion vacancies and interstitial vanadium ions (Watanabe, Andersson, Gjönnes & Terasaki, 1974; Morinaga & Cohen, 1976). An ordered structure has been detected in the composition range $VO_{1.2}$–$VO_{1.3}$ (Magnéli *et al.*, 1958; Westman & Nordmark, 1960; Westman, 1960; Andersson & Gjönnes, 1970; Bell & Lewis, 1971). As the oxygen sublattice is almost completely filled in this composition range, it has been suggested that the