The Origin Dependence of the Wyckoff Site Description of a Crystal Structure

By L. L. Boyle and J. E. Lawrenson

University Chemical Laboratory, Canterbury, Kent, England

When describing a crystal structure in terms of the Wyckoff sites occupied, equivalent alternatives often arise because the choice of origin of coordinates is subject to arbitrariness remaining within the standard choice in *International Tables for X-ray Crystallography*. The problem is explained and simple tables which enable any crystal structure to be described in any of the alternative ways are presented. Reference is made to the analogous problem in the theory of lattice complexes.

Introduction

One of the neatest generally applicable descriptions of a crystal structure is to specify the space group and then the occupation of the sets of equivalent sites, denoted by their Wyckoff (1922) label. Specification of the actual coordinates of the atoms within the unit cell then becomes redundant since these may be found by reference to Vol. I of *International Tables for X-ray Crystallography* (Henry & Lonsdale, 1969) provided that, for sites with degrees of freedom, the necessary parameters have been specified.

In this way the structure of caesium chloride is fully described by the space group O_h^1 with the caesium ions occupying the (a) sites and the chloride ions occupying the (b) sites, or *vice versa*. Both (a) and (b) sites have O_h point symmetry and are entirely equivalent; indeed the structure may be regarded as the interpenetration of two equal simple cubic lattices respectively specified by the cations and anions. In the same way the (c) and (d) sites are mutually equivalent: occupation of a (c) site may equally well be redescribed by occupation of a (d) site. If, however, the structure of the ordered phase of the intermetallic compound $AuCu_3$ is described in this way then the space group is O_h^1 with the gold atoms on the (a) sites and the copper atoms on the (c) sites, but the only equivalent redescription of the structure is that in which the gold atoms occupy the (b) sites and the copper atoms the (d) sites. Indeed the structure in which (a) and (d), or equivalently (b) and (c), sites are occupied is quite different, in fact that of rhenium trioxide, ReO_3. The reason for this restriction on the Wyckoff site description of a crystal structure is that in moving the (a) sites to the positions occupied by the (b) sites, which may be effected by an origin shift of $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, the (c) sites necessarily undergo this origin shift also and thus become (d) sites.

Theory

The general problem underlying the above illustration concerns the determination of all allowed origin shifts and the effect of each of these on all the Wyckoff sites

possible in a given space group. Two or more sets of sites will be said to be physically equivalent if

(i) they have the same point-group symmetry;

(ii) the orientations of the symmetry elements in the site groups with respect to the unit cell are the same: these have been elucidated by Boyle (1971);

(iii) they cannot be interrelated by space inversion only, *i.e.* there are not enantiomorphous pairs of sites;

(iv) the conditions limiting possible X-ray reflexions are the same;

(v) the environment of symmetry elements is identical.

Conditions (i) to (iv) are easily recognized from Table 4.3 of Vol. I of *International Tables for X-ray Crystallography* (Henry & Lonsdale, 1969) and the tables of Boyle (1971); condition (v) is best tested by trial and error. The test consists of applying the origin shift that interconverts sets satisfying (i) to (iv) and ensuring that every other set is either unchanged or converted into another physically equivalent set in the space group. Thus in D_{2h}^{27} the sets of sites (a) and (b) satisfy (i) to (iv) but the origin shift $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ which interconverts them does not leave the unique set (c) invariant and hence these sites do not satisfy condition (v). It is relevant to add at this point that for a set with one or more degrees of freedom an origin shift may leave the set invariant, provided that the value of the arbitrary parameter is subjected to the appropriate linear transformation; the precise transformations will not be specified in this paper but they can be deduced when necessary. In certain cases, *e.g.* D_{6h}^4, an allowed origin shift causes interchange of the labels of the arbitrary parameters in the set containing two degrees of freedom: this is irrelevant since the set is independent of the labelling of the parameters provided that these are given the appropriate numerical values. Occasionally, where origin shifts in perpendicular directions affect different sites, there is complete interchangeability of equivalent sites. Thus in D_2^2 a shift $(0\frac{1}{2}0)$ interchanges (a) and (b) only while the shift $(\frac{1}{2}00)$ interchanges (c) and (d) only; the values of the arbitrary parameters in the unchanged sites are, however, affected.

Of the 230 space groups, 159 allow an origin-depen-

dent choice of Wyckoff-site description. However, since the Wyckoff labelling of the sites is independent of the setting in the monoclinic groups, the choice of origin or the use of rhombohedral or hexagonal axes, the Tables presented in this paper are applicable to any of these standard variants given in *International Tables*.

Lattice complexes

A problem analogous to that discussed above may be posed in the theory of the description of a crystal structure in terms of lattice complexes. These were originally defined by Niggli (1919) as what is now known as a set of Wyckoff sites and it was recognized that lattice complexes were related on ascent and descent in symmetry within a given crystal system. Hermann (1935) felt that a more useful definition would be to ascribe different sets of Wyckoff sites to the same lattice complex if they could 'be transformed into one another by any rotations or changes of scale whatever, provided that the corresponding crystal system and the direction of its axes is not altered thereby'. The advantage of this was that the lattice-complex description was now invariant for different choices of the coordinate axes but Hermann did admit that a certain degree of abstraction had been incurred ('The definition ... is not so directly related to the coordinate representation as that of Niggli, since the symbols giving the relationship of the cell of the lattice complex to that of the space group *is not obvious*'). The idea was that the sets of Wyckoff sites were now merely concrete representations of the abstract lattice complex. However, Hermann's (1935) tables classified some enantiomorphous sets of sites as belonging to the same lattice complex (*e.g.* in T_d^6), while others (*e.g.* in O^8) belonged to different lattice complexes. Donnay, Hellner & Niggli (1966) proposed that enantiomorphous sets should belong to the same lattice complex but at the same time, following Hermann (1960), established a whole system of different superscripts to distinguish the different rep-

resentations of a lattice complex which, as can be seen from Table 1 of Hellner (1965), was merely tantamount to relabelling the Wyckoff sites in a complicated notation which sometimes gave information on ascent and descent in symmetry. Indeed, Hellner's (1965) paper shows the fundamental weakness of the description of a crystal structure by means of lattice complexes since in describing the structure of zinc blende (Space group T_d^2; Zn on (*a*), S on (*c*) *or* Zn on (*b*), S on (*d*) *or* Zn on (*c*), S on (*b*) *or* Zn on (*d*) S on (*a*) the lattice complex description becomes *FF″ or F′F′″ or F′F″ or F′F′″*. Although the last two might more logically be written *F″F′* and *F′″F′*, there is still no explanation of the restriction on the possible combinations of *F*-type lattice complexes. Presumably the conclusion was reached by translating the Wyckoff-site description. The four alternatives can be read off immediately from Table 7 below. Indeed since Tables 1–7 specify precisely the permutability of the Wyckoff sites there now seems to be little value in retaining the concept of a lattice complex in view of these defects.

The Tables

Tables 1–7 contain explicitly the allowed permutations of the Wyckoff sites for the space groups (classified according to crystal systems). The allowed permutations are specified by the rows of the Tables and the

Table 1. *Correlation of equivalent Wyckoff site descriptions for the triclinic space groups*

$$S_2^1 \quad \begin{vmatrix} a & b & c & d & e & f & g & h \\ b & a & g & f & h & d & c & e \\ c & g & a & e & d & h & b & f \\ d & f & e & a & c & b & h & g \\ e & h & d & c & a & g & f & b \\ f & d & h & b & g & a & e & c \\ g & c & b & h & f & e & a & d \\ h & e & f & g & b & c & d & a \end{vmatrix}$$

C_1^1: – No alternatives.

Table 2. *Correlation of equivalent Wyckoff site descriptions for the monoclinic space groups*

$$C_{1h}^1, C_2^3 \quad \begin{vmatrix} a & b \\ b & a \end{vmatrix} \qquad C_{2h}^1 \quad \begin{vmatrix} a & b & c & d & e & f & g & h & i & j & k & l & mn \\ b & a & f & e & d & c & h & g & i & j & k & l & nm \\ c & f & a & g & h & b & d & e & k & l & i & j & mn \\ d & e & g & a & b & h & c & f & j & i & l & k & mn \\ e & d & h & b & a & g & f & c & j & i & l & k & nm \\ f & c & b & h & g & a & e & d & k & l & i & j & nm \\ g & h & d & c & f & e & a & b & l & k & j & i & mn \\ h & g & e & f & c & d & b & a & l & k & j & i & nm \end{vmatrix}$$

$$C_{2h}^3 \quad \begin{vmatrix} a & b & c & d & e & f & g & h \\ b & a & d & c & e & f & g & h \\ c & d & a & b & f & e & h & g \\ d & c & b & a & f & e & h & g \end{vmatrix} \qquad C_{2h}^4 \quad \begin{vmatrix} a & b & c & d & e & f \\ b & a & d & c & f & e \\ c & d & a & b & e & f \\ d & c & b & a & f & e \end{vmatrix}$$

$$C_2^1, C_{2h}^2, C_{2h}^5 \quad \begin{vmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{vmatrix} \qquad C_{2h}^6 \quad \begin{vmatrix} a & b & c & d \\ b & a & d & c \end{vmatrix}$$

$C_{1h}^2, C_{1h}^3, C_{1h}^4, C_2^2$: – No alternatives.

Table 3. *Correlation of equivalent Wyckoff site descriptions for the orthorhombic space groups*

C_{2v}^1
```
a b c d e f g h
b a d c f e g h
c d a b e f h g
d c b a f e h g
```

C_{2v}^3
```
a b c d
b a d c
c d a b
d c b a
```

C_{2v}^{14}, D_{2h}^8
```
a b d e
b a e d
```

D_{2h}^{20}
```
a b c d e f i j
b a d c f e j i
```

D_2^1
```
a b c d e f g h i j k l m n o p q r s t
b a e f c d h g i j k l o p m n r q t s
c e a g b h d f k l i j m n o p s t q r
d f g a h b c e j i l k n m p o q r s t
e c b h a g f d k l i j o p m n t s r q
f d h b g a e c j i l k p o n m r q t s
g h d c f e a b l k j i n m p o s t q r
h g f e d c b a l k j i p o n m t s r q
```

$D_2^2, D_{2h}^{10}, D_{2h}^{13}, D_{2h}^{22}$
```
a b c d
a b d c
b a c d
b a d c
```

D_2^6
```
a b c d e f g h i j
b a d c e f g h j i
c d a b f e h g j i
d c b a f e h g i j
```

D_2^7
```
a b c d e f g h i j
b a d c e f g h i j
c d a b j i h g f e
d c b a j i h g f e
```

D_2^8
```
a b c d e f g h i j
b a d c e f h g j i
c d a b f e h g i j
d c b a f e g h j i
```

D_{2h}^1
```
a b c d e f g h i j k l m n o p q r s t u v w x y z
b a d c f e h g i j k l o p m n s t q r v u w x y z
c d a b g h e f j i l k n m p o q r s t u v w x z y
d c b a h g f e j i l k p o n m s t q r v u w x z y
e f g h a b c d k l i j m n o p r q t s u v x w y z
f e h g b a d c k l i j o p m n t s r q v u x w y z
g h e f c d a b l k j i n m p o r q t s u v x w z y
h g f e d c b a l k j i p o n m t s r q v u x w z y
```

D_{2h}^2
```
a b c d e f g h i j k l
a b c d f e g h i j k l
b a d c e f g h j i l k
b a d c f e g h j i l k
c d a b e f h g j i k l
c d a b f e h g j i k l
d c b a e f h g i j l k
d c b a f e h g i j l k
```

D_{2h}^3
```
a b c d e f g h i j k l m n o p
b a d c h g f e j i l k n m p o
c d a b g h e f j i k l o p m n
d c b a f e h g i j l k p o n m
```

D_{2h}^7, D_{2h}^{12}
```
a b c d e f
b a d c e f
c d a b f e
d c b a f e
```

D_{2h}^4
```
a b c d e f g h i j k l
b a d c e f g h i j l k
c d a b f e h g j i l k
d c b a f e h g j i k l
```

D_{2h}^5
```
a b c d e f g h i j
b a d c f e g h j i
c d a b e f h g i j
d c b a f e h g j i
```

D_{2h}^9
```
a b c d e f g h
b a d c e f h g
c d a b f e g h
d c b a f e h g
```

D_{2h}^{19}
```
a b c d e f g h i j k l p q
b a d c e f g h i j l k p q
c d a b f e h g j i l k q p
d c b a f e h g j i k l q p
```

D_{2h}^{21}
```
a b c d e f h i j k
b a d c f e i h k j
```

D_{2h}^{24}, D_{2h}^{28}
```
a b c d
b a d c
```

D_{2h}^{25}
```
a b c d e f g h i j
b a d c f e h g i j
c d a b f e g h j i
d c b a e f h g j i
```

D_{2h}^{26}
```
a b c d h i
b a d c i h
```

$C_{2v}^2, C_{2v}^4, C_{2v}^6, C_{2v}^8, C_{2v}^{10}, C_{2v}^{11}, C_{2v}^{13}, C_{2v}^{15}, C_{2v}^{20}, C_{2v}^{21}$
$D_2^3, D_{2h}^6, D_{2h}^{11}, D_{2h}^{14}, D_{2h}^{15}, D_{2h}^{16}, D_{2h}^{17}, D_{2h}^{18}, D_{2h}^{23}$
```
a b
b a
```

$C_{2v}^5, C_{2v}^7, C_{2v}^9, C_{2v}^{12}, C_{2v}^{16}, C_{2v}^{17}, C_{2v}^{18}, C_{2v}^{19}, C_{2v}^{22}, D_2^4, D_2^5, D_2^9, D_{2h}^{27}$: – No alternatives.

Table 4. *Correlation of equivalent Wyckoff site descriptions for the trigonal space groups*

$C_3^1, C_{3v}^1, C_{3v}^3$
$$\begin{array}{ccc} a & b & c \\ b & c & a \\ c & a & b \end{array}$$

D_3^1
$$\begin{array}{ccccccccccc} a & b & c & d & e & f & g & h & i & j & k \\ b & a & d & c & f & e & g & h & i & k & j \\ c & d & e & f & a & b & h & i & g & j & k \\ d & c & f & e & b & a & h & i & g & k & j \\ e & f & a & b & c & d & i & g & h & j & k \\ f & e & b & a & d & c & i & g & h & k & j \end{array}$$

D_3^2, S_6^1
$$\begin{array}{cccc} a & b & e & f \\ b & a & f & e \end{array}$$

$D_3^3, D_3^4, D_3^5, D_3^6$
$$\begin{array}{cc} a & b \\ b & a \end{array}$$

D_3^7, S_6^2
$$\begin{array}{cccc} a & b & d & e \\ b & a & e & d \end{array}$$

D_{3d}^1
$$\begin{array}{cccccc} a & b & c & d & f & g & i & j \\ b & a & d & c & g & f & j & i \end{array}$$

D_{3d}^2
$$\begin{array}{cc} c & d \\ d & c \end{array}$$

D_{3d}^3
$$\begin{array}{cccccc} a & b & e & f & g & h \\ b & a & f & e & h & g \end{array}$$

D_{3d}^5
$$\begin{array}{cccccc} a & b & d & e & f & g \\ b & a & e & d & g & f \end{array}$$

$C_3^2, C_3^3, C_3^4, C_{3v}^2, C_{3v}^4, C_{3v}^5, C_{3v}^6, D_{3d}^4, D_{3d}^6$: – No alternatives.

Table 5. *Correlation of equivalent Wyckoff site descriptions for the tetragonal space groups*

S_4^1
$$\begin{array}{cccccc} a & b & c & d & e & f \\ b & a & d & c & e & f \\ c & d & a & b & f & e \\ d & c & b & a & f & e \end{array}$$

S_4^2
$$\begin{array}{cccccc} a & b & c & d & e & f \\ b & a & d & c & e & f \\ c & d & b & a & f & e \\ d & c & a & b & f & e \end{array}$$

C_{4h}^1
$$\begin{array}{cccccccc} a & b & c & d & e & f & g & h & j & k \\ b & a & d & c & f & e & g & h & k & j \\ c & d & a & b & e & f & h & g & j & k \\ d & c & b & a & f & e & h & g & k & j \end{array}$$

C_{4h}^2
$$\begin{array}{cccccccc} a & b & c & d & e & f & g & h \\ b & a & d & c & f & e & h & g \end{array}$$

C_{4h}^3, C_{4v}^7
$$\begin{array}{cccc} a & b & d & e \\ b & a & e & d \end{array}$$

$C_{4h}^4, C_{4h}^6, D_{2d}^9, D_{4h}^{19}$
$$\begin{array}{cccc} a & b & c & d \\ b & a & d & c \end{array}$$

C_{4v}^1, D_4^2, D_4^6
$$\begin{array}{cccc} a & b & e & f \\ b & a & f & e \end{array}$$

D_{2d}^1
$$\begin{array}{cccccccccccc} a & b & c & d & e & f & g & h & i & j & k & l \\ b & a & d & c & f & e & h & g & j & i & l & k \\ c & d & a & b & f & e & g & h & k & l & i & j \\ d & c & b & a & e & f & h & g & l & k & j & i \end{array}$$

D_{2d}^5
$$\begin{array}{cccccccccc} a & b & c & d & e & f & h & i & j & k \\ b & a & d & c & f & e & h & i & k & j \\ c & d & a & b & f & e & i & h & k & j \\ d & c & b & a & e & f & i & h & j & k \end{array}$$

D_{2d}^2
$$\begin{array}{cccccccccccc} a & b & c & d & e & f & g & h & i & j & k & l \\ c & d & a & b & f & e & i & j & g & h & l & k \end{array}$$

D_{2d}^6, D_{2d}^7
$$\begin{array}{cccccc} a & b & c & d & g & h \\ b & a & d & c & h & g \end{array}$$

D_{2d}^8
$$\begin{array}{cccccc} a & b & c & d & f & g \\ b & a & d & c & g & f \end{array}$$

D_{2d}^{10}
$$\begin{array}{cccccccc} a & b & c & d & e & f & g & h \\ d & c & b & a & h & g & f & e \end{array}$$

D_{2d}^{11}, D_{4h}^{14}
$$\begin{array}{cccc} a & b & f & g \\ b & a & g & f \end{array}$$

D_4^1
$$\begin{array}{cccccccccccccc} a & b & c & d & e & f & g & h & j & k & l & m & n & o \\ b & a & d & c & f & e & g & h & k & j & n & o & l & m \\ c & d & a & b & e & f & h & g & j & k & o & n & m & l \\ d & c & b & a & f & e & h & g & k & j & m & l & o & n \end{array}$$

D_4^5, D_{4h}^9
$$\begin{array}{cccccccccccc} a & b & c & d & e & f & g & h & j & k & l & m \\ b & a & d & c & f & e & h & g & m & l & k & j \end{array}$$

D_4^9
$$\begin{array}{cccc} a & b & h & i \\ b & a & i & h \end{array}$$

D_{4h}^1
$$\begin{array}{cccccccccccccc} a & b & c & d & e & f & g & h & j & k & l & mn & o & p & q & s & t \\ b & a & d & c & f & e & g & h & k & j & ml & o & n & q & p & s & t \\ c & d & a & b & e & f & h & g & j & k & n & o & l & mp & q & t & s \\ d & c & b & a & f & e & h & g & k & j & o & n & ml & q & p & t & s \end{array}$$

D_{4h}^2
$$\begin{array}{cccccccc} a & b & c & d & g & h & k & l \\ c & d & a & b & h & g & l & k \end{array}$$

D_{4h}^3
$$\begin{array}{cccccccccc} a & b & c & d & e & f & i & j & k & l \\ b & a & d & c & f & e & j & i & l & k \end{array}$$

D_{4h}^4, D_{4h}^{17}
$$\begin{array}{cccc} a & b & i & j \\ b & a & j & i \end{array}$$

D_{4h}^5
$$\begin{array}{cccccccc} a & b & c & d & g & h & i & j \\ b & a & d & c & h & g & j & i \end{array}$$

D_{4h}^7
$$\begin{array}{cccccc} a & b & d & e & g & h \\ b & a & e & d & h & g \end{array}$$

D_{4h}^{10}
$$\begin{array}{cccccccc} a & b & c & d & g & h & i & j & l & m \\ a & b & c & d & g & h & j & i & l & m \\ c & d & a & b & h & g & i & j & ml \\ c & d & a & b & h & g & j & i & ml \end{array}$$

D_{4h}^{12}
$$\begin{array}{cccccccc} a & b & e & f & i & j & k & l \\ b & a & f & e & j & i & l & k \end{array}$$

D_{4h}^{16}
$$\begin{array}{cccc} c & d & g & h \\ d & c & h & g \end{array}$$

$C_4^1, C_4^3, C_{4h}^5, C_{4v}^3, C_{4v}^5, C_{4v}^8, D_{2d}^3, D_4^4, D_{2d}^{12}, D_{2d}^3, D_4^7, D_4^{10}, D_{4h}^6, D_{4h}^{15}$
$$\begin{array}{cc} a & b \\ b & a \end{array}$$

$C_4^2, C_4^4, C_4^5, C_4^6, C_{4v}^2, C_{4v}^4, C_{4v}^6, C_{4v}^9, C_{4v}^{10}, C_{4v}^{11}, C_{4v}^{12}, D_4^3, D_4^8, D_{4h}^8, D_{4h}^{11}, D_{4h}^{13}, D_{4h}^{18}, D_{4h}^{20}$: – No alternatives.

Table 6. *Correlation of equivalent Wyckoff site descriptions for the hexagonal space groups*

C^1_{3h}
$$\begin{vmatrix} a & b & c & d & e & f & g & h & i & j & k \\ b & a & d & c & f & e & g & h & i & k & j \\ c & d & e & f & a & b & h & i & g & j & k \\ d & c & f & e & b & a & h & i & g & k & j \\ e & f & a & b & c & d & i & g & h & j & k \\ f & e & b & a & d & c & i & g & h & k & j \end{vmatrix}$$

D^1_{3h}
$$\begin{vmatrix} a & b & c & d & e & f & g & h & i & l & m \\ b & a & d & c & f & e & g & h & i & m & l \\ c & d & e & f & a & b & h & i & g & l & m \\ d & c & f & e & b & a & h & i & g & m & l \\ e & f & a & b & c & d & i & g & h & l & m \\ f & e & b & a & d & c & i & g & h & m & l \end{vmatrix}$$

D^2_{3h}
$$\begin{vmatrix} a & b & c & d & e & f & g & h & i \\ c & d & e & f & a & b & h & i & g \\ e & f & a & b & c & d & i & g & h \end{vmatrix}$$

$D^3_{3h},\ C^1_{6h}$
$$\begin{vmatrix} a & b & c & d & f & g & j & k \\ b & a & d & c & g & f & k & j \end{vmatrix}$$

D^1_6
$$\begin{vmatrix} a & b & c & d & f & g & j & k & l & m \\ b & a & d & c & g & f & k & j & m & l \end{vmatrix}$$

$D^4_{3h},\ C^2_{6h},\ D^6_6,\ D^4_{6h}$
$$\begin{vmatrix} c & d \\ d & c \end{vmatrix}$$

$D^4_6,\ D^5_6$
$$\begin{vmatrix} a & b & c & d & g & h & i & j \\ b & a & d & c & h & g & j & i \end{vmatrix}$$

D^1_{6h}
$$\begin{vmatrix} a & b & c & d & f & g & j & k & l & m & p & q \\ b & a & d & c & g & f & k & j & m & l & q & p \end{vmatrix}$$

$C^1_6,\ C^2_6,\ C^3_6,\ C^4_6,\ C^5_6,\ C^6_6,\ C^1_{6v},\ C^2_{6v},\ C^3_{6v},\ C^4_{6v},\ D^2_6,\ D^3_6,\ D^2_{6h},\ D^3_{6h}$: – No alternatives.

Table 7. *Correlation of equivalent Wyckoff site descriptions for the cubic space groups*

T^1
$$\begin{vmatrix} a & b & c & d & f & g & h & i \\ b & a & d & c & i & h & g & f \end{vmatrix}$$

$T^2,\ T^2_d$
$$\begin{vmatrix} a & b & c & d & f & g \\ b & a & d & c & f & g \\ c & d & b & a & g & f \\ d & c & a & b & g & f \end{vmatrix}$$

$T^1_d,\ T^5_d$
$$\begin{vmatrix} a & b & c & d & f & g \\ b & a & d & c & g & f \end{vmatrix}$$

T^4_d
$$\begin{vmatrix} c & d & g & h \\ d & c & h & g \end{vmatrix}$$

T^1_h
$$\begin{vmatrix} a & b & c & d & e & f & g & h & j & k \\ b & a & d & c & h & g & f & e & k & j \end{vmatrix}$$

T^2_h
$$\begin{vmatrix} b & c \\ c & b \end{vmatrix}$$

$T^3_h,\ T^6_h,\ T^7_h,\ O^6,\ O^7$
$$\begin{vmatrix} a & b \\ b & a \end{vmatrix}$$

$T^4_h,\ O^4,\ O^7_h$
$$\begin{vmatrix} a & b & c & d \\ b & a & d & c \end{vmatrix}$$

T^5_h
$$\begin{vmatrix} d & e \\ e & d \end{vmatrix}$$

O^1
$$\begin{vmatrix} a & b & c & d & e & f & i & j \\ b & a & d & c & f & e & j & i \end{vmatrix}$$

O^2
$$\begin{vmatrix} b & c & e & f & i & j & k & l \\ c & b & f & e & j & i & l & k \end{vmatrix}$$

O^3
$$\begin{vmatrix} a & b & g & h \\ b & a & h & g \end{vmatrix}$$

O^1_h
$$\begin{vmatrix} a & b & c & d & e & f & i & j & k & l \\ b & a & d & c & f & e & j & i & l & k \end{vmatrix}$$

O^3_h
$$\begin{vmatrix} c & d & g & h \\ d & c & h & g \end{vmatrix}$$

O^4_h
$$\begin{vmatrix} b & c & i & j \\ c & b & j & i \end{vmatrix}$$

O^5_h
$$\begin{vmatrix} a & b & h & i \\ b & a & i & h \end{vmatrix}$$

$T^3,\ T^4,\ T^5,\ T^3_d,\ T^6_d,\ O^5,\ O^8,\ O^2_h,\ O^6_h,\ O^8_h,\ O^9_h,\ O^{10}_h$: – No alternatives.

correlations by the columns. In the first row and first column the relevant sites appear in alphabetical order. Sites which are invariant to all allowed origin shifts are omitted. Space groups of a given crystal system having the same correlation tables have been collected together to save space; no other similarity between the nature of the sites or the space groups is implied as Wyckoff's system of labelling is essentially an arbitrary cataloguing of the sets of special positions. As an illustrative example the spinel structure [O^7_h, Mg on (a), Al on (d), O on (e)] may be considered. According to Table 7, when (a) → (b), (d) → (c) and (e) is unchanged since it is not included. However the (e) sites do have one degree of freedom and inspection of *International Tables* (Henry & Lonsdale 1969) p. 340 shows that the new parameter x' is related to the original one x by the equation: $x' = x - \frac{1}{2}$. The alternative description is therefore O^7_h, Mg on (b), Al on (c), O on (e) with $x' = x - \frac{1}{2}$.

References

BOYLE, L. L. (1971). *Acta Cryst.* A27, 76–79.
DONNAY, J. D. H., HELLNER, E. & NIGGLI, A. (1966). *Z. Kristallogr.* 123, 255–262.
HELLNER, E. (1965). *Acta Cryst.* 19, 703–712.
HENRY, N. F. M. & LONSDALE, K. (Eds.) (1969). *International Tables for X-ray Crystallography*, Vol. I. *Symmetry Groups.* Birmingham: Kynoch Press.
HERMANN, C. (1935). *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, Band I. *Gruppentheoretische Tafeln.* Chap. 8. Berlin: Borntraeger.
HERMANN, C. (1960). *Z. Kristallogr.* 113, 142–154.
NIGGLI, P. (1919). *Geometrische Kristallographie des Diskontinuums.* Leipzig: Borntraeger.
WYCKOFF, R. W. G. (1922). *Mem. Carnegie Inst. Wash.* 318.