breadth which may amount to several percent. However this is an increase which results from a spreading out at the base of peak, it is not the kind of increase in breadth which we normally look for in comparing two peaks. The breadth at half maximum intensity represents more closely the quantity which is used in practice. Although there is a small increase in this kind of breadth, the magnitude is too small to be of importance or to be experimentally observable.

I am indebted to Dr B. D. Cullity for a preliminary discussion of powder pattern broadening by temperature vibration.

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# Some Comments on and *Addenda* to the Tables of Irreducible Representations of the Classical Space Groups Published by S. C. Miller and W. F. Love

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A summary is given of some work which has been performed to identify those special points, lines, and planes of symmetry that have been omitted from published tables of irreducible representations of space groups. In order to have a complete set of all the irreducible representations of every space group, it is necessary to determine the irreducible representations for these additional wave vectors in order to supplement the existing published sets of tables. The generation of these supplementary tables is reported.

## 1. Introduction

The irreducible representations of space groups have been used for many years for labelling the electronic band structures of crystalline solids. More recently, their use has been extended to labelling phonon dispersion relations and the energy eigenstates for other particles or quasi-particles. In addition to providing a useful scheme for labelling energy bands or dispersion relations, the irreducible representations of the space groups can also be used to predict essential degeneracies, to simplify the calculation of electronic band structures or of phonon dispersion relations, and in the determination of selection rules for processes involving electrons or phonons in crystalline solids; for details see, for example, Cracknell (1974, 1975).

Tables of irreducible representations were first published for three important symmorphic space groups, $Pm3m(O_h^1)$, $Fm3m(O_h^5)$, and $Im3m(O_h^9)$ by Bouckaert, Smoluchowski & Wigner (1936) and for two of the more important non-symmorphic space groups, $P6_3/mmc(D_{6h}^4)$ and $Fd3m(O_h^7)$, by Herring (1942). Since then, many papers have been published giving tables of the irreducible representations of various selections of space groups. During the last few years there have been several systematic attempts to publish complete sets of tables of irreducible representations for all the 230 classical space groups (Faddeyev, 1964; Kovalev, 1965; Miller & Love, 1967; Zak, Casher, Glück & Gur, 1969; Bradley & Cracknell, 1972). Some recent work which we have been doing, in connexion with the reduction of Kronecker products of space-group representations, has made us realize that each of these published sets of tables contains some deficiencies. We shall concern ourselves primarily with the tables of Miller & Love (1967), which we shall refer to hereafter as M & L, because they are the most explicit tables and also, being computer-generated, they are in the most convenient form for use in further computer-based calculations.

The points that we wish to make concern (i) the completeness of the identification of special points and lines of symmetry, without restrictions being imposed on the axial ratios for certain space groups (see § 2), (ii) the systematic identification of planes of symmetry in all space groups (see § 3), and (iii) the determination of the irreducible representations for all distinct wave vectors in the 'representation domain', $\Phi$, which for many space groups is larger than the 'basic domain', $\Omega$.

In the space available in this journal we shall only be able to summarize our work on these topics. There are, inevitably, a considerable number of new diagrams and tables that we have had to construct but which cannot be included here.*

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* The diagrams and tables are all included in a paper. *On the completeness of tables of irreducible representations of the classical space groups* (Davies & Cracknell, 1976).

## 2. Special points and lines of symmetry

Brillouin zones for the various space groups are illustrated on pages I24–I31 of M & L. However, for certain space groups the appearance of the Brillouin zone may be different for different values of the axial ratios. In each such case M & L only considered one of the possible sets of axial ratios. Thus, for example, the Brillouin zone used by M & L for the orthorhombic $C$ space groups is reproduced in Fig. 1($a$). In fact this diagram corresponds to $b>a$. In the tables of M & L any given orthorhombic $C$ space group is only considered in one orientation, relative to the chosen $x$, $y$, and $z$ axes. It is therefore necessary, for completeness, to consider the possibility $b<a$ as well; this leads to a Brillouin zone with a rather different appearance which is illustrated in Fig. 1($b$). Many of the special points and lines of symmetry are common to both diagrams. However, there are two lines of symmetry, labelled $F$ and $G$ in Fig. 1($b$) which are not present in Fig. 1($a$) and which were not included in the tables of M & L. Since these lines of symmetry do not pass through $\Gamma$, the determination of the irreducible representations for these wave vectors is not entirely trivial. Similar cases of restrictions on the axial ratios apply to several other Brillouin zones illustrated by M & L, see Table 1. Other possible restrictions on the axial ratios are indicated in the right-hand part of Table 1 and the corresponding illustrations were given in the book by Bradley & Cracknell (1972), which we shall refer to as B & C. We have determined the irreducible representations for these additional wave vectors.

## 3. Planes of symmetry

Suppose that we consider two space groups $\mathbf{G}_0$ and $\mathbf{G}$, which are based on the same Bravais lattice and which have isogonal point groups $\mathbf{P}_0$ and $\mathbf{P}$, respectively, where $\mathbf{P}_0$ is the holosymmetric point group of that crystal system and $\mathbf{P}$ is a subgroup of $\mathbf{P}_0$. We shall refer to a space group as a *holosymmetric* space group if its isogonal point group is the holosymmetric point group of the appropriate crystal system. Thus $\mathbf{G}_0$ is a holosymmetric space group but $\mathbf{G}$ is not. In the construction of tables of space-group representations, both by M & L and by B & C, the treatment of planes of symmetry for any given space group varied according to whether the space group is a holosymmetric space group or not.

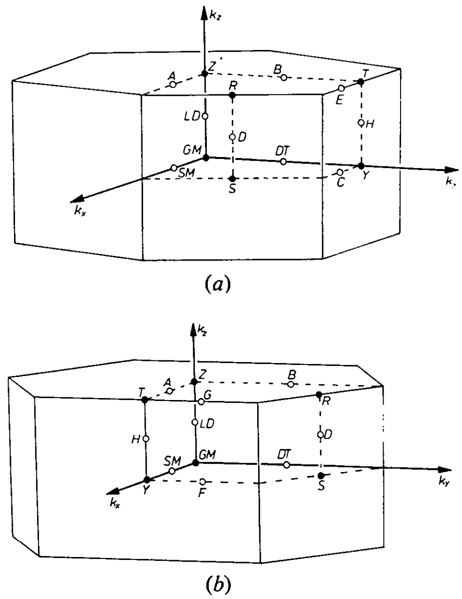


Fig. 1. Brillouin zone for orthorhombic, $C$, space groups, ($a$) $b>a$, and ($b$) $b<a$.

Table 1. *Restrictions on axial ratios for diagrams of Brillouin zones*

| Bravais Lattice | Restrictions | Fig. of M & L | Fig. of B & C | Other possible restrictions | Fig. of B & C |
|---|---|---|---|---|---|
| Triclinic, $P$ | * | 2 | – | Unrestricted | 3·2 |
| Monoclinic, $P$ | * | 3 | – | Unrestricted | 3·3 |
| Monoclinic, $B$ ($C$) | * | 4 | – | Unrestricted | 3·4 |
| Orthorhombic, $P$ | None | 5 | 3·5 | – | – |
| Orthorhombic, $C$ | $b>a$ | 6 | 3·6 ($b$) | $b<a$ | 3·6 ($a$) |
| Orthorhombic, $F$ | $1/a^2>1/b^2+1/c^2$ | 7 | 3·8 ($d$) | $1/b^2>1/c^2+1/a^2$ | 3·8 ($c$) |
| | | | | $1/c^2>1/a^2+1/b^2$ | 3·8 ($b$) |
| | | | | $\left.\begin{array}{l}1/a^2<1/b^2+1/c^2\\1/b^2<1/c^2+1/a^2\\1/c^2<1/a^2+1/b^2\end{array}\right\}$ | 3·8 ($a$) |
| Orthorhombic, $I$ | $a>b>c$ or $a>c>b$ | 8 | 3·7 ($a$) | $b>a>c$ or $b>c>a$ | 3·7 ($b$) |
| | | | | $c>b>a$ or $c>a>b$ | 3·7 ($c$) |
| Tetragonal, $P$ | None | 9 | 3·9 | – | – |
| Tetragonal, $I$ | $a>c$ | 10 | 3·10 ($a$) | $a<c$ | 3·10 ($b$) |
| Cubic, $P$ | None | 11 | 3·13 | – | – |
| Cubic, $F$ | None | 12 | 3·14 | – | – |
| Cubic, $I$ | None | 13 | 3·15 | – | – |
| Trigonal, $R$ | $a>\sqrt{2}c$ | 14 | 3·11 ($a$) | $a<\sqrt{2}c$ | 3·11 ($b$) |
| Hexagonal, $P$ | None | 15 | 3·12 | – | – |

* For triclinic and monoclinic lattices the restrictions are complicated. This difficulty is avoided by B & C by using the fundamental unit cell in place of the Wigner–Seitz unit cell in the definition of a Brillouin zone.

For each holosymmetric space group the wave vectors corresponding to special points of symmetry and lines of symmetry were identified by M & L and by B & C. But if $\mathbf{k}_0$ is a wave vector which describes a *plane* of symmetry in a holosymmetric space group $\mathbf{G}_0$, then $\mathbf{k}_0$ was deliberately omitted from both sets of tables. If $\mathbf{k}_0$ is a wave vector which describes a plane of symmetry in $\mathbf{G}$, which is not a holosymmetric space group, then $\mathbf{k}_0$ may or may not be included in those tables. If $\mathbf{k}_0$ corresponds to a *plane* of symmetry in $\mathbf{G}$ and the same $\mathbf{k}_0$ also corresponds to a *plane* of symmetry in $\mathbf{G}_0$ then $\mathbf{k}_0$ was omitted from the tables for $\mathbf{G}$. However, if $\mathbf{k}_0$ corresponds to a *plane* of symmetry in $\mathbf{G}$ but corresponds to a *point* or *line* of symmetry in $\mathbf{G}_0$, then $\mathbf{k}_0$ was included in the tables for $\mathbf{G}$. The reasons for this apparently rather arbitrary distinction between the treatment of different planes of symmetry are historical; they are connected with the manner in which the tables were constructed and the purposes for which it was originally expected that the tables would be used. Thus, because there is no logical reason for excluding the planes of symmetry and because in many cases the planes of symmetry have become more important in practice, we propose that for a complete identification of all the irreducible representations of the space groups all the planes of symmetry should be included in the tables for each space group. We have constructed the additional tables that are necessary for this, using the format of the tables of M & L.

## 4. Representation domain and basic domain

We first remind our readers of the definitions of the terms 'basic domain' and 'representation domain' (Bradley, Wallis & Cracknell, 1970; Bradley & Cracknell, 1972):

(1) For each Brillouin zone there is a *basic domain*, $\Omega$, such that $(\sum_R R\Omega)$ is equal to the whole Brillouin zone, where $R$ are the elements of the holosymmetric group, $\mathbf{P}_0$, of the appropriate crystal system.

(2) For each space group there is a representation domain, $\Phi$, of the appropriate Brillouin zone, such that $(\sum_R R\Phi)$ is equal to the whole Brillouin zone, where the sum over $R$ runs through the elements of the isogonal point group, $\mathbf{P}$, of that space group.

For each of the holosymmetric space groups $\Phi$ can be taken to be identical with $\Omega$. But for the remaining space groups the volume of $\Phi$ is some small-integer multiple of the volume of $\Omega$.

The importance of the representation domain, $\Phi$, lies in the fact that to determine *all* the (induced) irreducible representations of a space group, $\mathbf{G}_0$ or $\mathbf{G}$, it is necessary to obtain the irreducible representations of one wave vector in every distinct star for that space group. The representation domain is the smallest fraction of the Brillouin zone which can be guaranteed to contain *at least one wave vector from every star.* However, the published sets of tables of space-group representations only give the irreducible representations for wave vectors within the basic domain, $\Omega$, and not necessarily throughout the whole of the representation domain, $\Phi$. It so happens that for every space group except one, it is possible to use a general procedure to determine the irreducible representations for a wave vector in ($\Phi$–$\Omega$) from those for some related wave vector in $\Omega$. The exception is the space group $Pa3(T_h^6)$, for which it is impossible to avoid some additional tabulation. An outline of the general procedure, as well as the inescapable additional tables for $Pa3(T_h^6)$, will be found in § 5.5 of B & C. We have now also made a detailed study of the representation domains for all the space groups, with particular reference to the problem of identifying for each space group those additional wave vectors in ($\Phi$–$\Omega$) which it is necessary to include in order to obtain one, and only one, wave vector of each star. The results of this work will be published elsewhere in due course.

## 5. Conclusion

In the tables* referred to in the *Introduction* we have tabulated the irreducible representations for all the additional special points and lines of symmetry mentioned in § 2 and for all the additional planes of symmetry mentioned in § 3. We also have in hand the preparation of tables identifying all the new wave vectors in the region ($\Phi$–$\Omega$) that belong to stars not included in $\Omega$ for each space group.

* See preceding footnote.

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