Acta Cryst. (1955). **8**, 595

Symmetry relations between structure factors.

By JÜRG WASER, *Department of Chemistry, The Rice Institute, Houston, Texas, U.S.A.*

(*Received* 12 *May* 1955)

It is known (Buerger, 1949) that the relationships between structure factors generated by space-group operations may be described by the use of the operations of the point group isomorphous with the space group considered, and of phase factors related to the translational components of the space-group elements. However, none of the existing space-group tables lists all independent relations, nor does there appear to exist a simple derivation of them (see, however, MacGillavry (1950) and Patterson (1952)). Such a derivation is given in the following, and an example provided.

Let C_j be any space-group operation relating the vector $\mathbf{r}$ to $C_j\mathbf{r} = \mathbf{t}_j + A_j.\mathbf{r}$, where $\mathbf{t}_j$ is the translational component of the operation and A_j is a dyadic corresponding to the proper or improper rotation isomorphous with C_j. The value of $\mathbf{t}_j$ depends on the position of the origin relative to the plane, axis, or center of A_j. For proper or improper rotations the conjugate dyadic A_{jC} is equal to the inverse dyadic A_j^{-1}, which relation insures invariance of distances (see, for example, Zachariasen (1945)).

Consider the structure factor

$$F_{\mathbf{h}} = \int_{\text{unit cell}} \varrho(\mathbf{r}) \exp(2\pi i \mathbf{h}.\mathbf{r}) dV ,$$

in usual notation. Since $\varrho(C_j\mathbf{r}) = \varrho(\mathbf{r})$,

$$F_{\mathbf{h}} = \int \varrho(\mathbf{r}) \exp[2\pi i(\mathbf{h}.C_j\mathbf{r})] dV$$
$$= \exp 2\pi i(\mathbf{h}.\mathbf{t}_j) \int \varrho(\mathbf{r}) \exp[2\pi i(\mathbf{h}.A_j.\mathbf{r})] dV .$$

The integral may be interpreted as structure factor $F_{\mathbf{h}^{(j)}}$, where $\mathbf{h}^{(j)} = \mathbf{h}.A_j = A_j^{-1}.\mathbf{h}$ is related to $\mathbf{h}$ by the inverse of the operation A_j.

Thus

$$F_{\mathbf{h}^{(j)}} = \exp(-2\pi i \mathbf{h}.\mathbf{t}_j) F_{\mathbf{h}} .$$

To obtain all independent relations between the structure factors only those operations C_j need be considered whose rotational components completely generate the point group isomorphous to the space group. This means that from a knowledge of the Hermann–Mauguin symbol all independent relations may be derived. If the symbol is redundant, relations which are dependent result.

The form of the relations depends on the choice of the origin. If the proper components of $\mathbf{t}_j$ are in doubt, consideration of the parameters related by the operation C_j will provide them, as will be apparent in the following example.

Example.—Space group $Pn3n$; origin at center of symmetry.

In self explanatory notation:

Type of operation	$C_j(x, y, z)$	$\mathbf{t}_j$	$F_{hkl} =$
$n_{[0,x,y]}$	$\bar{x}, \frac{1}{2}+y, \frac{1}{2}+z$	$0, \frac{1}{2}, \frac{1}{2}$	$(-1)^{k+l}F_{\bar{h}kl}$
$3_{[x,x,x]}$	y, z, x	$0, 0, 0$	F_{lhk}
$n_{[x,x,z]}$	$\frac{1}{2}+y, \frac{1}{2}+x, \frac{1}{2}+z$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$(-1)^{h+k+l}F_{khl}$
$4_{[\frac{1}{2},\frac{1}{2},z]}$	$\frac{1}{2}-y, x, z$	$\frac{1}{2}, 0, 0$	$(-1)^{h}F_{k\bar{h}l}$
$4_{[\frac{1}{2},\frac{1}{2},z]}$	$y, \frac{1}{2}-x, z$	$0, \frac{1}{2}, 0$	$(-1)^{k}F_{\bar{k}hl}$

Since the point group isomorphous with $Pn3n$ contains 47 operations different from identity there will be 47 relations among structure factors. However, only the relations of the first three lines of the table are independent: for instance, those of lines 4 and 5 follow from combination of lines 2 and 3, while $F_{hkl} = F_{\bar{h}\bar{k}l}$ is a consequence of lines 1 and 2. Note the importance, in lines 4 or 5, of the fact that the indices hkl are related by the dyadic inverse to the one which (except for $\mathbf{t}_j$) relates the parameters. Since line 5 deals with the inverse of the operation of line 4 the indices $k\bar{h}l$ on line 4 are related to hkl in the same way as the parameters on line 5 are related to x, y, z (except for $\mathbf{t}_j$), and inversely.

References

BUERGER, M. J. (1949). *Proc. Nat. Acad. Sci., Wash.* **35**, 198.

MACGILLAVRY, C. M. (1950). *Acta Cryst.* **3**, 214.

PATTERSON, A. L. (1952). 'Symmetry Maps Derived from the $|F|^2$ Series' in *Computing Methods and the Phase Problem in X-ray Crystal Analysis* (R. Pepinsky, Editor). State College: X-ray Crystal Analysis Laboratory.

ZACHARIASEN, W. H. (1945). *Theory of X-ray Diffraction in Crystals*, Appendix A. New York: Wiley.

Acta Cryst. (1955). **8**, 595

The accuracy of structures determined by powder methods, with reference to the Ag–Zn ζ structure.

By I. G. EDMUNDS, *Physics Department, College of Technology, Manchester* 1, *England*

(*Received* 26 *May* 1955)

It is gratifying to find that the qualitative X-ray examination carried out by Bergman & Jaross (1955) on powder specimens and on orientated aggregates of 'single crystal' domains leads to an approximate structure for the Ag–Zn ζ phase which, in so far as it goes, is in agreement with the more detailed structure given by Edmunds & Qurashi (1951) and based on measured intensities of X-ray powder reflexions. Nevertheless, the