1.4. Symmetry in reciprocal space

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With Appendix A1.4.2 by U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve

1.4.1. Introduction

Crystallographic symmetry, as reflected in functions on reciprocal space, can be considered from two complementary points of view.

(1) One can assume the existence of a certain permissible symmetry of the density function of crystalline (scattering) matter, a function which due to its three-dimensional periodicity can be expanded in a triple Fourier series (*e.g.* Bragg, 1966), and inquire about the effects of this symmetry on the Fourier coefficients – the structure factors. Since there exists a one-to-one correspondence between the triplets of summation indices in the Fourier expansion and vectors in the reciprocal lattice (Ewald, 1921), the above approach leads to consequences of the symmetry of the density function which are relevant to the representation of its Fourier image in reciprocal space. The symmetry properties of these Fourier coefficients, which are closely related to the crystallographic experiment, can then be readily established.

This traditional approach, the essentials of which are the basis of Sections 4.5–4.7 of Volume I (*IT* I, 1952), and which was further developed in the works of Buerger (1949, 1960), Waser (1955), Bertaut (1964) and Wells (1965), is one of the cornerstones of crystallographic practice and will be followed in the present chapter, as far as the basic principles are concerned.

(2) The alternative approach, proposed by Bienenstock & Ewald (1962), also presumes a periodic density function in crystal space and its Fourier expansion associated with the reciprocal. However, the argument starts from the Fourier coefficients, taken as a discrete set of complex functions, and linear transformations are sought which leave the magnitudes of these functions unchanged; the variables on which these transformations operate are h, k, l and φ – the Fourier summation indices (*i.e.*, components of a reciprocal-lattice vector) and the phase of the Fourier coefficient, respectively. These transformations, or the groups they constitute, are then interpreted in terms of the symmetry of the density function in direct space. This direct analysis of symmetry in reciprocal space will also be discussed.

We start the next section with a brief discussion of the point-group symmetries of associated direct and reciprocal lattices. The weighted reciprocal lattice is then briefly introduced and the relation between the values of the weight function at symmetry-related points of the weighted reciprocal lattice is discussed in terms of the Fourier expansion of a periodic function in crystal space. The remaining part of Section 1.4.2 is devoted to the formulation of the Fourier series and its coefficients (values of the weight function) in terms of space-group-specific symmetry factors. Section 1.4.3 then explains the basis for an automated generation of simplified geometrical structure-factor formulae, which are presented for all the two- and three-dimensional space groups in Appendix 1.4.3. This is a revised version of the structure-factor tables given in Sections 4.5–4.7 of Volume I (*IT* I, 1952). Appendix 1.4.4 contains a reciprocal-space representation of the 230 crystallographic space groups and some explanatory material related to these space-group tables is given in Section 1.4.4; the latter are interpreted in terms of the two viewpoints discussed above. The tabular material given in this chapter is compatible with the direct-space symmetry tables given in Volume A (*IT* A, 1983) with regard to the space-group settings and choices of the origin.

Most of the tabular material, the new symmetry-factor tables in Appendix 1.4.3 and the space-group tables in Appendix 1.4.4 have been generated by computer with the aid of a combination of numeric and symbolic programming techniques. The algorithm underlying this procedure is briefly summarized in Appendix 1.4.1. Appendix 1.4.2 deals with computer-adapted space-group symbols, including the set of symbols that were used in the preparation of the present tables.

Computer generation of symmetry information is not new. However, we can quote the Bilbao Crystallographic Server (*e.g.* Aroyo *et al.*, 2006) as a rich source of symmetry information which is readily accessible from the Internet.

1.4.2. Effects of symmetry on the Fourier image of the crystal

1.4.2.1. Point-group symmetry of the reciprocal lattice

Regarding the reciprocal lattice as a collection of points generated from a given direct lattice, it is fairly easy to see that each of the two associated lattices must have the same point-group symmetry. The set of all the rotations that bring the direct lattice into self-coincidence can be thought of as interchanging equivalent families of lattice planes in all the permissible manners. A family of lattice planes in the direct lattice is characterized by a common normal and a certain interplanar distance, and these two characteristics uniquely define the direction and magnitude, respectively, of a vector in the reciprocal lattice, as well as the lattice line associated with this vector and passing through the origin. It follows that any symmetry operation on the direct lattice must also bring the reciprocal lattice into self-coincidence, *i.e.* it must also be a symmetry operation on the reciprocal lattice. The roles of direct and reciprocal lattices in the above argument can of course be interchanged without affecting the conclusion.

The above elementary considerations recall that for any point group (not necessarily the full point group of a lattice), the operations which leave the lattice unchanged must also leave unchanged its associated reciprocal. This equivalence of point-group symmetries of the associated direct and reciprocal lattices is fundamental to crystallographic symmetry in reciprocal space, in both points of view mentioned in Section 1.4.1.

With regard to the effect of any given point-group operation on each of the two associated lattices, we recall that:

(i) If P is a point-group rotation operator acting on the direct lattice (*e.g.* by rotation through the angle α about a given axis), the effect of this rotation on the associated reciprocal lattice is that of applying the inverse rotation operator, P^{-1} (*i.e.* rotation through $-\alpha$ about a direction parallel to the direct axis); this is readily found from the requirement that the scalar product $\mathbf{h}^T \mathbf{r}_L$, where $\mathbf{h}$ and $\mathbf{r}_L$ are vectors in the reciprocal and direct lattices, respectively, remains invariant under the application of a point-group operation to the crystal.

(ii) If our matrix representation of the rotation operator is such that the point-group operation is applied to the direct-lattice (column) vector by *premultiplying* it with the matrix P, the corresponding operation on the reciprocal lattice is applied by *postmultiplying* the (row) vector $\mathbf{h}^T$ with the point-group rotation matrix. We can thus write, *e.g.*, $\mathbf{h}^T \mathbf{r}_L = (\mathbf{h}^T P^{-1})(P\mathbf{r}_L) = [(P^{-1})^T \mathbf{h}]^T (P\mathbf{r}_L)$. Note, however, that the orthogonality relation-

references