THE DEGREES OF FREEDOM OF SIMPLE SYMMETRY OPERATIONS*

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ABSTRACT

The geometrical dimensions of elements of symmetry, symmetry operations and symmetrical patterns are shown to be correlated. It is argued that the conventional elements of symmetry are strictly applicable only to three dimensional patterns, their use in defining one- and two-dimensional groups resulting in ambiguity. The specific elements of one- and two-dimensional groups are defined.

Point symmetry groups define the symmetry of the environment of a point (for instance, the center of an ideal crystal form) by means of elements of symmetry containing the given point. In defining *spacial* point symmetry groups, we use only five types of elements of symmetry, the center of symmetry (C_i), the plane of symmetry (C_s), axes of rotation (C_n), and axes of rotary-reflection (S_n) or axes of rotary-inversion (J_n). The latter two are interchangeable *complex* elements of symmetry. We will here consider only the three *simple* elements C_i, C_s, and C_n. These elements are symbols indicating the admissibility of specific symmetry operations. Thus C_i indicates the operation of inversion, C_s indicates reflection, and C_n indicates rotation through angles of 360°/n. These elements, however, are more than mere symbols; they *control* the corresponding symmetry operation. This control can be expressed in the following law of degrees of freedom of simple symmetry operations.

$a+b=c$.
a = number of geometrical dimensions of the element of symmetry.
b = degrees of freedom (= dimensions) of the controlled symmetry operation.
c = number of geometrical dimensions of the pattern under consideration.

C_i is a (dimensionless) point. It controls the operation of inversion, consisting in moving points along lines passing through the center of symmetry. There is no restriction on the direction of these lines, therefore the operation of inversion has *three* degrees of freedom.

C_n is one-dimensional. In the operation of rotation, points are able to move only in planes normal to C_n; the operation of rotation has *two* degrees of freedom.

C_s is two-dimensional. The corresponding operation consists in the transfer of points from one side of the plane to the other. Visualizing the operation, we see that all points move along parallel lines normal to the

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plane of symmetry. The operation of reflection has only *one* degree of freedom.

Thus C_i, C_s, C_n, and the corresponding operations satisfy the law of degrees of freedom. That this law is not a truism becomes clear when we consider the symmetry of one- and two-dimensional patterns.

It is customary to define the two-dimensional *plane* point symmetry groups (for instance the symmetry of crystal faces) by means of the corresponding spacial point groups, all the elements of a group lying normal to the plane pattern. Only three types of groups fulfill this requirement, namely C_n, C_s, and C_{nv}. We cannot, however, legitimately exclude C_i. The law of degrees of freedom shows that this method of defining plane point symmetry groups is arbitrary, the arbitrariness residing in the choice of one additional dimension for the sake of convenience. We could quite as legitimately choose to define plane patterns in terms of the symmetry elements of four or more dimensional spaces. The inconsistency in the use of three dimensions to define the symmetry of two-dimensional patterns results in one ambiguity, namely the equivalence of C_i and C_2. Now the essence of inversion is the establishment of enantiomorphic equivalents, and that of rotation the establishment of congruent equivalents. Thus the equivalence of C_i and C_2 is inadmissible.

The discrepancy resulting from recourse to more dimensions than necessary is even more striking in the case of the one-dimensional *linear* point symmetry groups. There are only two such groups, one being asymmetric. In terms of spacial groups the other can be defined by any of three, in this case equivalent, elements, namely C_i, C_s, or C_2.

The above considerations are of no practical consequence; we shall continue to state crystal face symmetries in terms of spacial point symmetry groups. Theoretically, however, the law of degrees of freedom of symmetry operations is a useful concept. It states that in choosing elements of symmetry we may not transcend the geometrical dimensions of the pattern under investigation if we wish to avoid ambiguity. C_i, C_s, and C_n then, are specifically elements of symmetry of three-dimensional groups, not admissible in one- and two-dimensional groups.

The element of symmetry specifically representing the single symmetrical linear symmetry point group is obviously a point, as we must claim the one available dimension to provide the degree of freedom of the corresponding operation. This operation is a reflection, in virtue of the single degree of freedom. It is a reflection in a point and the controlling point of reflection may be symbolized as A_s. A_1 designates the asymmetric linear point symmetry group. The edges between crystal faces, for instance, belong either to the group A_1 or A_s.

Plane point symmetry groups define two-dimensional patterns. The two possible specific elements of symmetry are the point rotation (B_n) and the line of reflection (B_s). The corresponding operations are rotation around a point (two degrees of freedom) and reflection in a line (one degree of freedom). The asymmetric group is given the symbol B_1. Thus plane point symmetry groups are restricted to B_1, B_n, B_s, and B_{ns}. These, of course, correspond to the Schoenflies symbols C_1, C_n, C_s, and C_{nv}.

The following figure shows the relations between the different elements of symmetry, the controlled operations, and the dimensions of the pattern.

Dimensions of Pattern	Name of Symmetry Groups	Dimensions of Element of Symmetry		
		0	1	2
1	Linear Point Symmetry Groups	Point of Reflection A_s ↘	—	—
2	Plane Point Symmetry Groups	Point of Rotation B_n ↘	Line of Reflection B_s ↘	—
3	Spacial Point Symmetry Groups	Point of Inversion C_i ↘	Line of Rotation C_n ↘	Plane of Reflection C_s ↘

Operation of Inversion
Three degrees of Freedom

Operation of Rotation
Two degrees of Freedom

Operation of Reflection
One degree of Freedom

Note: The figure suggests an interesting extrapolation, namely expansion downward and to the right into the domain of four- and more-dimensional spaces. Should the extrapolation be valid, then the elements of symmetry of four-dimensional space, for instance, would be as follows:

(1) Point of ?.
(2) Line of inversion.
(3) Plane of rotation.
(4) Three-dimensional space of reflection.