

About the concept and definition of “noncrystallographic symmetry”

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Abstract. The definition of “noncrystallographic symmetry” given in Volume B of the *International Tables for Crystallography* actually corresponds to the concept of “local symmetry”. A new definition of “noncrystallographic symmetry” is proposed, which fully complies with that of “crystallographic symmetry” in Volume A of the *International Tables for Crystallography*.

The concept of “noncrystallographic symmetry” is, quite obviously, directly related to that of “crystallographic symmetry” so that once a definition of the latter is given, that of the former is obtained spontaneously. This is probably the reason why no explicit definition of “noncrystallographic symmetry” is given in Volume A of the *International Tables for Crystallography*. Even the concept of noncrystallographic point groups, presented in section 10.1.4, is introduced without an explicit definition but only as the groups differing from the crystallographic point groups presented in Sections 10.1.2 and 10.1.3.

As a matter of fact, one should not even need an explicit definition of “noncrystallographic symmetry” once that of “crystallographic symmetry” is given. Unfortunately, in the literature, and especially in the structural biology literature, the term “noncrystallographic symmetry” is used in a manner in striking contrast with what is directly implied by the definition of “crystallographic symmetry”. This contradiction is so fundamental that it causes serious misunderstandings and misinterpretations. We will show that the use of “noncrystallographic symmetry” in structural biology is inconsistent with the accepted definition of

“crystallographic symmetry” and suggest that an alternative terminology should be used.

To understand the problem let us start with the definition of “crystallographic symmetry operations” given in [1] Section 8.1.5:

A motion is called a crystallographic symmetry operation if a crystal pattern exists for which it is a symmetry operation.

A *motion* is an isometry, a transformation keeping angles and distances unchanged, *i.e.* a transformation without deformation. A *crystal pattern* is the extension of a crystal structure to a periodic arrangement of whatever object, concrete or abstract, constitutes the structure. The atoms forming a crystal structure represent a special case of a crystal pattern. This definition applies to the n -dimensional Euclidean space E^n and can be expressed in a quantitative way with the aid of group theory. With respect to a basis of E^n , the symmetry operations of the space group of the crystal pattern are represented by $(n + 1) \times (n + 1)$ augmented matrices where the top-left $n \times n$ block represents the linear part of the operation (the part that leaves the origin fixed) and the additional column represents the vector part of the operation (the part which gives the translation component of the symmetry operation). The above definition of a crystallographic symmetry operation implies that with respect to a suitable basis of E^n (namely a primitive basis of the periodic pattern) the linear part of the matrix representing the operation is an integral matrix. In E^2 and E^3 this results in the well-known *crystallographic restriction* according to which only rotations (direct or inverse) of order 1, 2, 3, 4 and 6 are compatible with the existence of a crystal pattern. This restriction is extended to include also operations of order 5, 8, 10 and 12 for the four-dimensional space [2].

By an obvious contraposition, one is led to the definition of a *noncrystallographic symmetry operation* as a motion for which *no* crystal pattern exists allowing this motion as a symmetry operation. In particular, in E^2 and E^3 , a noncrystallographic symmetry operation is a motion whose linear part is different from rotations (direct or inverse) of order 1, 2, 3, 4 and 6, and in E^4 different also from order 5, 8, 10 and 12.

In the structural biology literature, however, a different definition is given for “noncrystallographic symmetry operation”, which clearly contradicts the official definition of “crystallographic symmetry operation” in [1]. This problematic definition is as follows [3]:

Crystallographic symmetry applies to the whole of the three-dimensional crystal lattice. Hence, the symmetry must be expressed both in the lattice and in the repeating pattern within the lattice. In contrast, noncrystallographic symmetry is valid only within a limited volume about the noncrystallographic symmetry element.

This use of the term *noncrystallographic symmetry* is improper and should be strongly discouraged not only because it contradicts the definition of crystallographic sym-

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metry in [1] but also because the concept covered by the definition is well-established under the term “**local symmetry**”. For a discussion of this concept in a more general context, see *e.g.* [4].

A symmetry operation acting on a “limited volume” differs from a space group operation not in the *nature* of the operation itself but because its action is limited to a subdomain of the crystal space. If the crystal space is partitioned into several (finitely or infinitely many) components S_i and $\Phi: S_i \rightarrow S_j$ is a motion transforming the component S_i into the component S_j , Φ in general is not a motion for the whole crystal space and therefore it is not one of the operations of the space group of the crystal, even when by its nature it is compatible with the existence of a crystal pattern, *i.e.* it obeys the crystallographic restriction. Such a motion is well known in mathematics: it is a *space groupoid operation* in the sense of Brandt¹ [5] and is called a *partial operation* (in contrast to *global*, or operation acting on the whole crystal space) [7]. It is not required that Φ brings S_j back onto S_i and in general it is not even defined for any component S_k different from S_i . Therefore a partial operation is not necessarily a symmetry operation, since that requires to map *every* element of the crystal pattern to another element of it. When $i = j$, *i.e.* when the operation $\Phi: S_i \rightarrow S_i$ brings a component to coincide with itself, the partial operation is of special type and is called *local* [8]. Also in this case, the operation Φ does not need to act on any component different from S_i and it may be crystallographic or noncrystallographic.

Summarizing, there are two almost independent concepts which are mixed up in the quoted definitions for “crystallographic symmetry” and “noncrystallographic symmetry”. On the one hand, a motion may or may not be crystallographic, depending on whether its linear part can be written as an integral matrix with respect to a suitable basis.

On the other hand, the action of a motion may or may not be restricted to a proper subdomain of the crystal space (*e.g.* a volume close to the symmetry element). But by restricting to a subdomain one will usually lose periodicity of the crystal pattern, therefore such partial/local operations may conform with the crystallographic restriction, but are not required to do so. For example, a rotation axis can be surrounded by n points mapped onto each other by an n -fold rotation. For a local operation acting only on the points close to the rotation axis, there is no restriction on n . For $n = 2, 3, 4, 6$ (in E^2 or E^3), the points can make part of a periodic pattern, for the other values of n they can not. But in any case, the definition in [3] would call the operation “noncrystallographic”.

For the reasons given, we propose to amend the problematic definition of noncrystallographic symmetry in [3] as follows:

A motion of E^n is called a noncrystallographic symmetry operation if there exists no n -dimensional crystal pattern for which it is a symmetry operation.

All reference to the domain of action of the motion should be excluded from the definition because this criterion differentiates a space group (containing only global operations) from a space groupoid (containing also partial/local operations).

The given definition is equivalent with the statement that the linear part of a noncrystallographic motion cannot be expressed as an integral matrix with respect to any chosen basis of E^n . It should be noted that the definition includes motions without fixed points, *i.e.* with a proper translational component. However, it is the very nature of a noncrystallographic symmetry operation, that the translational components can never give rise to a discrete periodic pattern.

Finally, we suggest to complement this definition with the following explicit statement:

A motion of E^n mapping onto itself a subdomain of a crystal pattern but not the whole crystal pattern is called a local symmetry operation. It may be crystallographic or noncrystallographic depending on whether or not it is possible to extend the subdomain to an n -dimensional crystal pattern invariant under the motion.

These two definitions dissolve the inconsistency with the accepted definition of “crystallographic symmetry” and at the same time conform with the well-established terminology for partial symmetries [5, 7, 8].

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¹ It is important to specify “in the sense of Brandt” because in the literature there is an alternative meaning of “groupoid” introduced by Hausmann & Ore [6], namely a set on which binary operations act, but neither the identity nor the inversion are included. This type of set is today called a *magma*.