Basic concepts of group theory in crystallography

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Introduction

Symmetry is one of the central concepts in crystallography. When you think about it, it is hard to expect that it could be any other way, because the very objects of crystallographic research, the crystals themselves, exhibit such remarkable perfection. Humans have been fascinated by the beauty of symmetry since the beginning of time, to the point that the symmetry has been considered beauty itself. This all shows that the appearance of symmetry in the world around us is connected deeply to the human experience of the universe.

But what has all this to do with purely mathematical subject of the theory of groups? What are groups anyway and what is their relationship with symmetry in general? In the lecture the emphasis will be on the notion that the group theory, in the crystallographic context, is merely a mathematical formalism that describes symmetry. Sometimes though, the rigour of the mathematical concepts tends to obscure the simplicity of the underlying principles. It is therefore beneficial to use more *visual approach* and let the natural human ability to apprehend symmetry do its work. Although group theory will be introduced in general terms, the two dimensional plane groups will be described in more detail. Plane groups are easily visualized and contain all the necessary formalism that can than readily be mentally extended to space groups that dictate the packing of molecules in crystals.

Group theory basics

The mathematical group is a set of elements that can be combined (in an operation) to yield new elements of the same set. But these elements and the operation between them, have to satisfy certain properties, called axioms of the group:

- **The existence of an identity element E** There exist an element E of the group G that leaves all other elements unchanged, i.e. AE = EA = A for every A in G.
- **The existence of an inverse element** For every element A in the group G there exists an element B such that AB=E. Than B is called an *inverse* of A, $B = A^{-1}$. Note that this does not exclude the possibility that $A=B=A^{-1}$, in other words that the element can be its own inverse.
- **Closure under the operation** Product of any two elements must also be an element of the group. That is for any elements A, and B of G, AB is also an element of G.
- **Associativity of the operation** The operation in the group must be associative, i.e. it must not be sensitive to the order in which it is carried out. For any three elements of the group it must be true that A(BC) = (AB)C.

It is immediately visible from the group axioms that they are postulated with symmetry in mind. If we look at some symmetric object, than the set of symmetry operations of that object form a group. Indeed, there is always an identity element which is equal to leaving object unchanged; for each symmetry operation there is another symmetry operation that returns the object to the original position, i.e. there is an inverse; applying two symmetry operations in succession is also a symmetry operation of the object; and finally the application of symmetry operations is associative. Therefore, each group actually shows some internal symmetry of the underlying set.

Let us mention some examples of sets that form groups. Number one and multiplication {1, ·} form a group, albeit a trivial one, group containing only an identity element. The set {1, -1} forms a group under multiplication, group of only two members. The number of elements of the group is called **order of a group**. But number one and addition do not form a group, {1, +}, as this is not closed under addition. But if we extend it to the set of all whole numbers {..., -2, -1, 0, 1, 2..., +} than we have a group. The set of all real numbers without 0 forms a group under multiplication. If we have any set of n elements than the set of all permutations of these elements forms a group, so called *symmetric group* S_n. We notice that groups can have finite and infinite number of elements.

Some important definitions

Probably the most important property of groups is that they can have **subgroups**. The subgroup H of group G is a subset of elements of G that itself forms a group. It is best illustrated by an example. Consider the symmetry elements of a equilateral triangle (Fig. 1), they form a group of order 6 and it is called D_3 (also called dihedral group; dihedral group of order n is a group of symmetries of regular n-gon). In crystallographic context this is also known as point group 32.

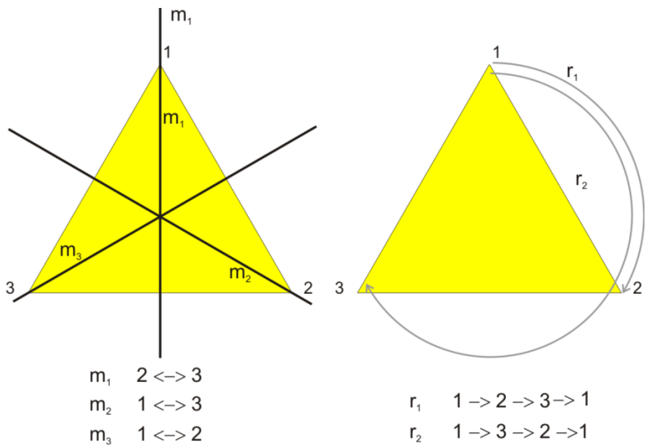

Figure 1. Symmetry elements of regular 3-gon, more commonly known as equilateral triangle ☺. On the left are three reflection lines, passing through point 1-3. On the right are two rotations by 120° (r_1) and 240° (r_2).

The group D_3 consists of the following six elements {e, m_1, m_2, m_3, , r_2}. Now let us take a look at these three elements of the D_3: identity element, rotation by 120° r_1 and rotation by 240° r_2. It can be seen that the rotations do not mix with the mirror elements, in other words, by rotating the triangle you can never get to the mirror image. In other words rotations form a subgroup 3 of the group D_3 (the order of the subgroup is 3, Table 1). Notice that reflections do not form a subgroup (for example the product of reflections $m_1 \cdot m_2 = r_2$ is a rotation). This also leads to the another important theorem (**Lagrange's theorem**) stating that the order of a group must be divisible by the order of any of it's subgroups. Therefore it is impossible for D_3 to have a subgroup of order 4, but possible for order 3, and it does! In fact rotations form something called **cyclic group**. In cyclic group each element of the group can be obtained just by repeatedly applying one element: r_1, $r_1 \cdot r_1 = r_2$, $r_1 \cdot r_1 \cdot r_1 = e$. Think of it in this way, we rotate by 120°, then rotate once more by 120°, and then once more and we are back where we were. One convenient way of representing the operation of the group is by so called **multiplication table (Cayley's table)**. The multiplication table of the group D_3 is given in Table 1.

Table 1. The multiplication table of the D_3 group. The concept of a subgroup is easily visible from the multiplication table, as the red square inside the blue one also forms a group. Note that the full group is non commutative, while the subgroup is commutative and cyclic.

	e	**r_1**	**r_2**	**m_1**	**m_2**	**m_3**
e	e	r_1	r_2	m_1	m_2	m_3
r_1	r_1	r_2	e	m_3	m_1	m_2
r_2	r_2	e	r_1	m_2	m_3	m_1
m_1	m_1	m_2	m_3	e	r_2	r_1
m_2	m_2	m_3	m_1	r_1	e	r_2
m_3	m_3	m_1	m_2	r_2	r_1	e

Group D_3 of order 6

Subgroup of order 3 (rotations only)

e	r_1	r_2
r_1	r_2	e
r_2	e	r_1

One other important thing to notice is that nowhere in the group axioms the commutativity was required, and indeed the application of symmetry elements is generally noncommutative. It would require that the multiplication table would have to be symmetric across the diagonal, which for group D_3 does not hold true (Table 1). As for the cyclic groups already mentioned, all the elements of the group can be generated by a subset of group elements, called **group generators**.

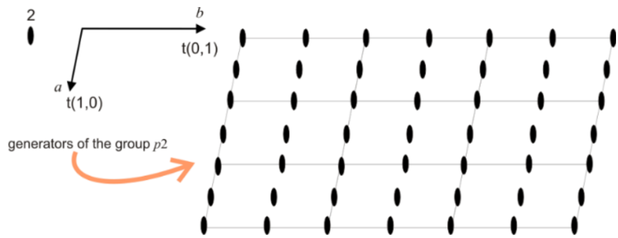

Figure 2. One example how an entire infinite plane group (in this case *p*2) can be generated just by three symmetry elements, one twofold rotation and two translations. They are called the generators of the group.

Groups in crystallography

In crystallographic context both the finite and infinite groups appear. **Point groups** are the groups that have at least one point not moved by any of the symmetry operations. In other words all symmetry elements of the point group intersect in one point. They are the example of finite groups. **Space groups** describe the full three-dimensional symmetry of the crystal. Space groups are an example of infinite groups. Loosely speaking, their infiniteness is „caused“ by translational symmetry. The group of translations forms a subgroup of a space group. Moreover, this subgroup is commutative and also a **normal subgroup**.

Visual approach to group theory

Having in mind the natural human ability to recognize symmetry, it is advantageous to make use o f it in the introduction to group theory concepts. By interactively drawing plane group patterns on the screen, one can more easily apprehend the mutual disposition of symmetry elements in various groups, and thus help the learning process (Figure 4).

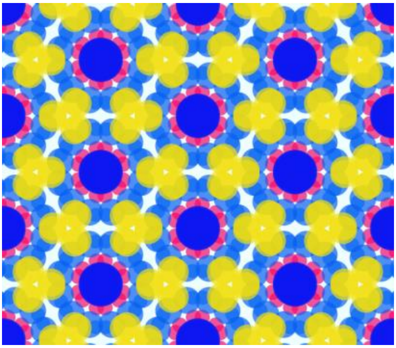

Figure 4. Interactive drawing of the symmetry patterns is not only instructive but also visually pleasing.

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