CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 20: The 10 2D Point Groups and Their Notations

In this lecture, we will look into developing all the possible two-dimensional point groups. These point groups will be composed of the five rotational symmetries $1, 2, 3, 4$, and 6, along with the mirror for the reflection symmetry.

Some of the point groups have already been partially developed. Let us first list the basic elements:

$$1, 2, 3, 4, 6, m$$

Based on these, we will develop all the point groups.

The first point group is simply the identity, or rotational symmetry 1. This can be illustrated graphically. Consider an arbitrary point and a reference line. Previously we used an asymmetric motif, but now we will use a standard symbol to depict the point groups in space groups. This symbol is a small circle.

Note: This circle should not be interpreted as a geometric circle. It represents an asymmetric motif, meaning the motif has no symmetry. We will use this symbol consistently for all point groups.

This is the first point group, where no symmetry operations are applied. The graphical illustration would be a single circle representing the asymmetric motif.

Next, consider a point group based on a two-fold rotational symmetry. Place the motif at some location. A two-fold rotation (180°) rotates the motif to a new position. This represents the point group based on a 2-fold rotation.

Similarly, a 3-fold rotational symmetry works as follows. Starting with the motif at one location, rotate through 120° to place the next motif, then another 120° for the next, and finally another 120° rotation returns to the starting position. This is the point group based on 3-fold rotational symmetry.

For a 4-fold rotational symmetry, starting with an asymmetric motif, rotate through 90° to place subsequent motifs. After four rotations of 90°, the motif returns to the original position. This represents the 4-fold point group.

Finally, the 6-fold rotational symmetry is illustrated by placing the motif, rotating 60° to place the next, and continuing this way through 6 positions, returning to the original location. This is the 6-fold point group.

Now consider reflection. Let there be a mirror plane and a motif on one side. The reflection operation brings the motif to the mirrored position. To indicate a change in handedness, we place a small comma inside the circle. If the first motif is right-handed, the reflected motif is left-handed. This represents the point group with reflection symmetry.

Next, we combine mirrors with rotational symmetries. Some cases have already been discussed:

- Mirror combined with 1-fold rotation has been illustrated.
- Mirror combined with 2-fold rotation: Place a mirror M_1 and an asymmetric motif. Rotate the motif 180°; the mirror reflects the motif with a change in handedness. Geometrically, a second mirror M_2 appears, and the handedness of the motifs is changed through M_2. This represents the point group combining a mirror with a 2-fold rotation.
- Mirror combined with 3-fold rotation: Place a mirror M_1. The threefold rotation rotates the motif and the mirror positions through angles of 120° to generate M_1, M_2, M_3. A left-handed motif is generated at each mirror position. Unlike the

2-fold case, no additional mirrors are created. This is an important point for notation of these point groups.

- Mirror combined with 4-fold rotation: This follows similarly, but with rotations of 90° and mirrors appearing at appropriate positions. The motifs' handedness is assigned accordingly.

Graphical representation of these point groups can be illustrated by placing the asymmetric motif (small circle) and drawing the positions after rotations and reflections. The commas inside the circles indicate handedness change due to reflections.

Now, consider the mirror combined with the four-fold rotational symmetry. The mirror will get rotated by the 4-fold rotation through 90°, so we have mirrors M_1 and M_2. Placing a motif, a 90° rotation brings it to the next position, another 90° rotation to the next, and another 90° rotation to the final position. Mirror operations are also applied, giving left-handed motifs at all four positions.

If we label the motifs as 1, 2, 3, and 4, motifs 1 and 4 are related through a mirror at an angle of 45°, and motifs 2 and 3 similarly. These additional mirrors can be labeled M_3 and M_4. This shows that additional mirrors are created in this case. All symmetry operations operate over the entire space, ensuring self-coincidence of motifs after transformations.

For six-fold rotational symmetry with a mirror, 60° rotations are used. Mirrors M_1, M_2, and M_3 are positioned appropriately. Placing the motifs, successive 60° rotations place the motifs at all six positions. The mirror operations generate left-handed motifs at all positions. Additional mirrors appear at angles corresponding to the relationships between motifs, labeled M_4, M_5, and M_6.

> Note: In the case of 3-fold rotation with a mirror, no additional mirrors are generated.

Counting all the point groups in 2 dimensions, we have 6 in the top row and 4 in the bottom row, giving a total of ***10 two-dimensional point groups***.

There are two methodologies for assigning notations to these point groups:

1. Schoenflies notation
2. Hermann-Mauguin (International) notation

Schoenflies Notation

- 1-fold rotation: C_1 (C stands for cyclic group, 1 for one-fold rotation (no symmetry)).
- 2-fold rotation: C_2
- 3-fold rotation: C_3
- 4-fold rotation: C_4
- 6-fold rotation: C_6
- Only reflection: C_s

For rotation with mirrors:

- 2-fold rotation + mirror: C_{2v}
    - 2 for 2-fold rotation, v for vertical mirror plane.
- 3-fold rotation + mirror: C_{3v}
- 4-fold rotation + mirror: C_{4v}
- 6-fold rotation + mirror: C_{6v}

Note: Starting with a horizontal mirror would lead to the same point group. Choice of mirror orientation affects notation only.

International (Hermann-Mauguin) Notation

- 1-fold rotation: 1

- 2-fold rotation: 2
- 3-fold rotation: 3
- 4-fold rotation: 4
- 6-fold rotation: 6
- Only mirror: m

For rotation + mirrors:

- 2-fold rotation + mirror: $2mm$
- 3-fold rotation + mirror: $3m$
- 4-fold rotation + mirror: $4mm$
- 6-fold rotation + mirror: $6mm$

These notations list all symmetry operations that independently generate the point group.

Let us explain the notations for the international (Hermann-Mauguin) system:

- In the case of 2-fold rotation with mirrors, the notation $2mm$ arises as follows:
    - 2 comes from the 2-fold rotation.
    - m_1 is the original mirror, and m_2 is generated by a combination of operations.
    - Therefore, we list both mirrors in the notation: $2mm$.
- For 3-fold rotation with a mirror, no additional mirrors are generated, so the notation is simply $3m$.
- For 4-fold rotation with mirrors, like the 2-fold case, additional mirrors are generated, giving the notation $4mm$.
- For 6-fold rotation with mirrors, additional mirrors are generated as well, giving the notation $6mm$.

Note: The international notation is generally used in crystallography. Schoenflies notation may be used occasionally, but most of the time we use the international notation for both 2D and 3D point groups.

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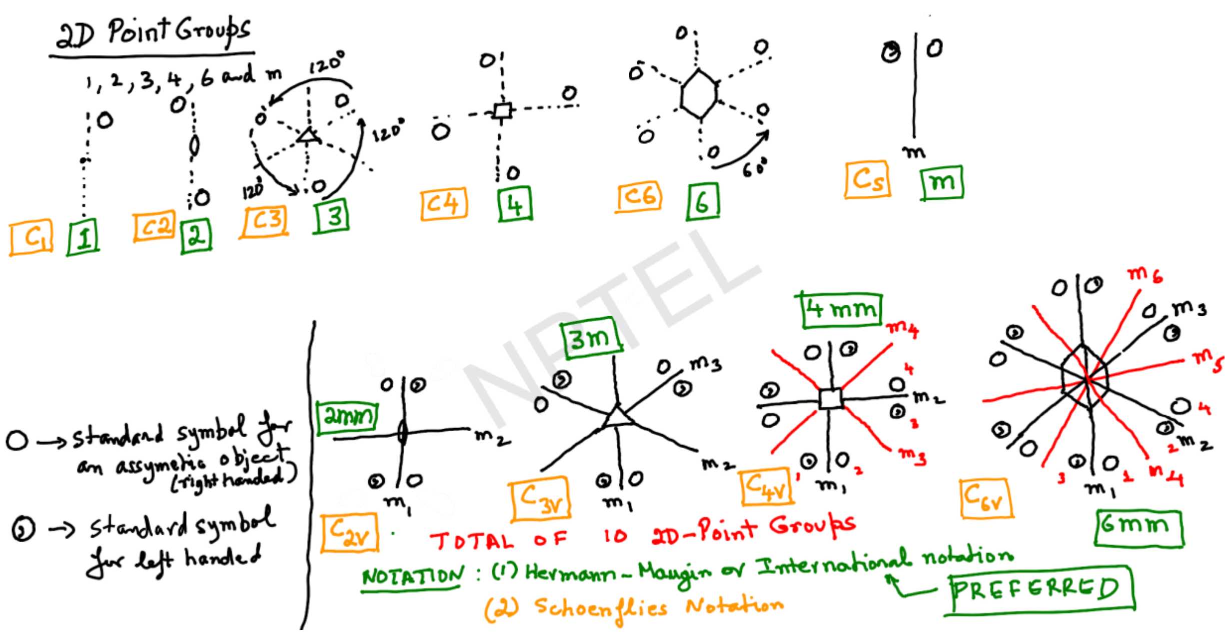

Example: Non-Crystallographic Point Group

Consider a 5-fold rotation with a mirror.

- Start with a mirror. A 72° rotation generates additional mirrors: M_1, M_2, M_3, M_4, and M_5, giving a total of 5 mirrors.
- The Schoenflies notation is C_{5v}.
- The international notation is $5m$.

Note: 5-fold rotational symmetry is not allowed in crystallography. This example is provided to illustrate that no additional mirrors are created in such a scenario. Placing motifs confirms this.

Exercise/Question

We have identified all 10 crystallographic point groups.

Consider two mirrors, M_1 and M_2, parallel to each other and separated by a distance a.

- Question: What is the result of the combination σ_1 followed by σ_2? What operation does this produce?

  Hint: Since the mirrors are not intersecting, this cannot be a point group. This leads to the topic of plane groups, where point groups are combined with translation symmetry.

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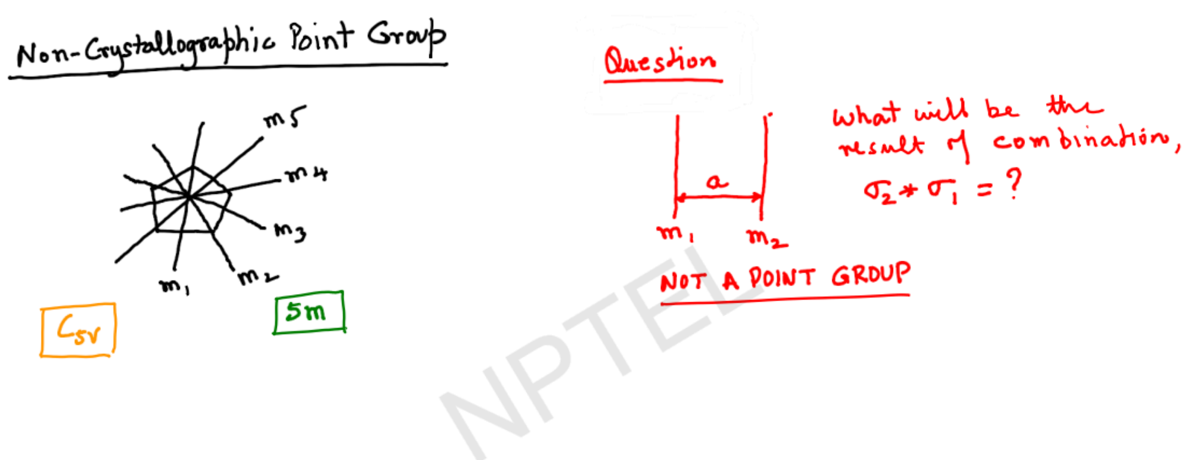

Thank you.