Crystallographic Groups

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1 Introduction

As the name suggests, the crystallographic groups deal with the structure of crystals, which are often described by their periodic nature. The subject has found its application in physics, most notably in the study of solid. Thus, we will restrict our analysis to three-dimensional space due to its practicality as well the easier visualizations and intuitions for the derivation which follows.

2 Preliminary

2.1 Transformation groups

Let G be a **transformation group** on the set X with the action by the group denoted by $\circ$, then for any $g, g_1, g_2 \in G$ and $x \in X$,

$$\begin{aligned} &g \circ x \in X, \\ &g_1 \circ (g_2 \circ x) = (g_1 g_2) \circ x, \\ &e \circ x = x, \end{aligned}$$

where e is the identity element of G.

Consider two elements x and y of X. we say that x is ***G*-equivalent** to y and denote by $x \sim y$ if there exists $g \in G$ such that $g \circ x = y$. In fact, $\sim$ defines an equivalence relation so we can partition X into equivalence classes; then, any element can only belong to one equivalence class. The equivalence class of x is called the **orbit** of x and denoted by

$$O_x = \{g \circ x \mid g \in G\} \subset X.$$

Let us also define the **stabilizer** of x, which is the set of all elements of G that leave x invariant. More explicitly, we write

$$G_x = \{g \in G \mid g \circ x = x\} \subset G.$$

It can be shown that G_x is a subgroup of G so we can apply the properties of subgroups (and their cosets) in group theory.

One useful result that we shall prove is stated as follows: Let G be a finite transformation group on X, then for any $x \in X$, one has

$$|O_x| = \frac{|G|}{|G_x|}.$$

First, consider $O_x = \{x\}$, then any element of G sends x to itself, so $G = G_x$ and the equality above trivially holds. If $|O_x| > 1$, consider $y \in O_x$ and different from x. There exists $g \in G$ such that $g \circ x = y$. For any $h \in G_x$, we have $(gh) \circ x = g \circ (h \circ x) = g \circ x = y$, so any element of the left coset gG_x sends x to y. Conversely, if there is some g' such that $g' \circ x = y$, then $g' \circ x = g \circ x$ or $(g^{-1}g') \circ x = x$, meaning that $g^{-1}g' \in G_x$ or $g' \in gG_x$. Hence, there is a one-to-one correspondence between the left coset gG_x and $y \in O_x$, so $|O_x|$ is equal to the number of left cosets of G_x (including G_x). Since each coset contains $|G_x|$ elements and any two different cosets of G_x do not intersect, we find the number of cosets to be $|G|/|G_x|$, and we again arrive at the above equality. □

Let us now focus on a subset Y of X. We define the ***G*-symmetry group** or just **symmetry group** of Y by

$$S = \{g \in G \mid g \circ Y = Y\}.$$

This means that any element of S either fixes Y or permutes the elements of Y. Then, if we start with the transformation group G, we want to find all the possible symmetry groups and the corresponding subsets of X that exhibit these symmetries. For our problem, Y is a subset of $\mathbb{R}^3$ and G is the Euclidean group in $\mathbb{R}^3$.

2.2 Euclidean group

We define the **Euclidean group** in $\mathbb{R}^n$, denoted by $E(n)$, by the group of all transformations that preserve the distance in $\mathbb{R}^n$, i.e., for any $A \in E(n)$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$,

$$\|A \circ \mathbf{x} - A \circ \mathbf{y}\| = \|\mathbf{x} - \mathbf{y}\|.$$

Let $T(n)$ be the **translation group** in $\mathbb{R}^n$ containing all translations on $\mathbb{R}^n$ and $R(n)$ be the **rotation group** in $\mathbb{R}^n$ containing all transformation that preserves the inner product $\langle \cdot, \cdot \rangle$ in $\mathbb{R}^n$. This corresponds to rotation (and inversion) of $\mathbb{R}^3$ about the origin, hence the name. It can be proven that

$$E(n) = T(n) \rtimes R(n).$$

Also, $R(n)$ is isomorphic to the **orthogonal group** in $\mathbb{R}^n$, $O(n)$, so we can identify any element of $R(n)$ by an $n \times n$ matrix of determinant ± 1.

For the case of $\mathbb{R}^3$, all non-trivial elements of $E(3)$ can be achieved by combining the following transformation:

- Translation by $\mathbf{d}$: $T_{\mathbf{d}}$,
- Rotation of angle θ about an axis $\hat{\mathbf{k}}$ passing through a fixed point $\mathbf{a}$: $R^{\mathbf{a}}(\theta\hat{\mathbf{k}})$,
- Inversion about a fixed point $\mathbf{b}$: $I^{\mathbf{b}}$.

We will also mention some important combinations that often appear in literature:

– Screw displacement: A rotation about an axis with a translation along that axis (in either order),

– Reflection in a plane†,

– Improper rotation†: A rotation about an axis with a reflection about the plane perpendicular to that axis (in either order),

– Glide plane operation: A reflection about a plane with a translation parallel to that plane (in either order).

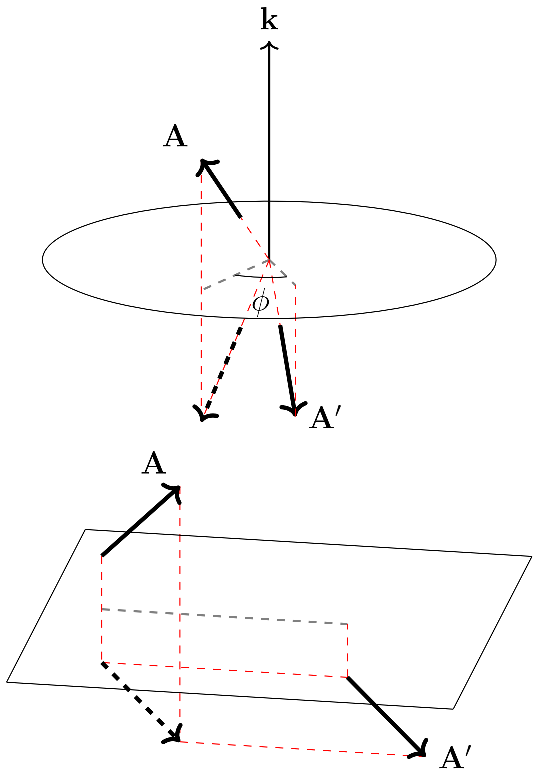


Figure 1: Examples of transformation of $\mathbf{A}$ to $\mathbf{A}'$. *Above*: An improper rotation. *Below*: A glide plane operation.

Also, consider two rotations of θ about $\hat{\mathbf{k}}$, one passes through the origin $\mathbf{O}$ and one passes through a fixed point $\mathbf{a}$, and similarly for inversions. If we denote $R(\theta\hat{\mathbf{k}}) = R^{\mathbf{O}}(\theta\hat{\mathbf{k}})$ and $I = I^{\mathbf{O}}$, it is easy to see that

$$R^{\mathbf{a}}(\theta\hat{\mathbf{k}}) = T_{\mathbf{a}} R(\theta\hat{\mathbf{k}}) T_{\mathbf{a}}^{-1},$$
$$I^{\mathbf{a}} = T_{\mathbf{a}} I T_{\mathbf{a}}^{-1},$$

by shifting the fixed point to the origin, performing the rotation, then shifting everything back. These form conjugacy classes so the rotation subgroup of $E(3)$ that fixes one point can always be identified with the rotation subgroup that fixes the origin, which is $R(3)$.

Since $R(3) \simeq O(3)$, we can represent any rotation by a matrix. It is sufficient to consider only one rotation about one particular axis because the matrix corresponding to another rotation about a different axis can be calculated by a change of basis. By convention, the z-axis is usually chosen, and the matrix corresponding to $R(\phi\hat{\mathbf{z}})$ is

$$R(\phi\hat{\mathbf{z}}) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Also, we would like to represent a reflection (instead of an inversion). A reflection about the xy plane is given by the matrix

$$M_{xy} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

We will use these results in section 4.

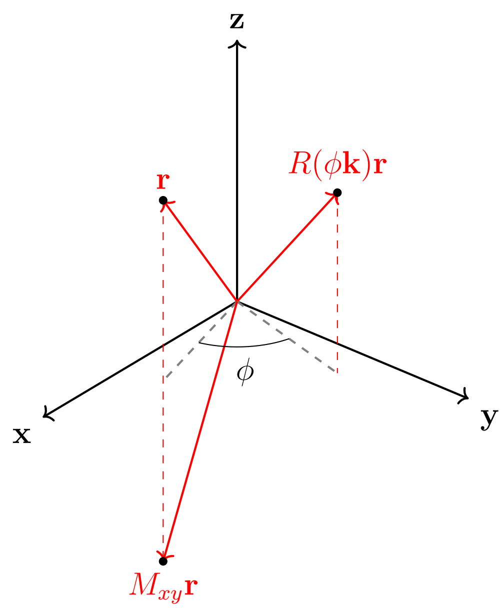


Figure 2: Rotation and reflection of a point located at $\mathbf{r}$

†Note: For general $R(n)$, the matrices with determinant 1 correspond to **(proper) rotations** while those with determinant -1 correspond to **improper rotations**. In 3D, any improper rotation can be achieved by a certain rotation and an inversion, so we can consider translation, rotation, and inversion as the three basic operations (this is not the case in 2D because an inversion is equivalent to a rotation by 180° so it does not include reflection).

2.3 Lattice

In this section, we try not to be too precise with the definitions and only give a qualitative picture of these concepts.

A **(three-dimensional) lattice** can be defined as a set

$$L = \{\mathbf{l} \in \mathbb{R}^3 \mid \mathbf{l} = m_1\mathbf{a_1} + m_2\mathbf{a_2} + m_3\mathbf{a_3}, m_i \in \mathbb{Z}\},$$

where $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$ are linearly independent vectors in $\mathbb{R}^3$. These are called the **primitive lattice vectors**. If we are given the set L, there can be different set of primitive lattice vectors that still span L so the choice for these vectors is not unique. We will regard the lattice as a set of *points* or *position vectors* in $\mathbb{R}^3$ called the **lattice points** and denote them by $\mathbf{l}_p$. When we speak of a *translation* or *displacement vector* with length and direction equal to an element of L, we will use the notation $\mathbf{l}$.

By dividing the whole space into repeated volumes with respect to the primitive lattice vectors, each volume becomes a **primitive unit cell**. Then, these unit cells must have the same shape, do not intersect with each other, cover all of $\mathbb{R}^3$, and we can always go from one unit cell to another by a translation $T_{\mathbf{l}}$ with $\mathbf{l} \in L$. Notice that in this definition, each unit cell contains only one lattice point, hence, the name *primitive*. We can also define a **non-primitive unit cell** by dividing the space with respect to $n_1\mathbf{a_1}, n_2\mathbf{a_2}, n_3\mathbf{a_3}$ where $n_1, n_2, n_3 \in \mathbb{N}^*$ and $(n_1, n_2, n_3) \neq (1, 1, 1)$. Then, each unit cell contains more than one lattice point.

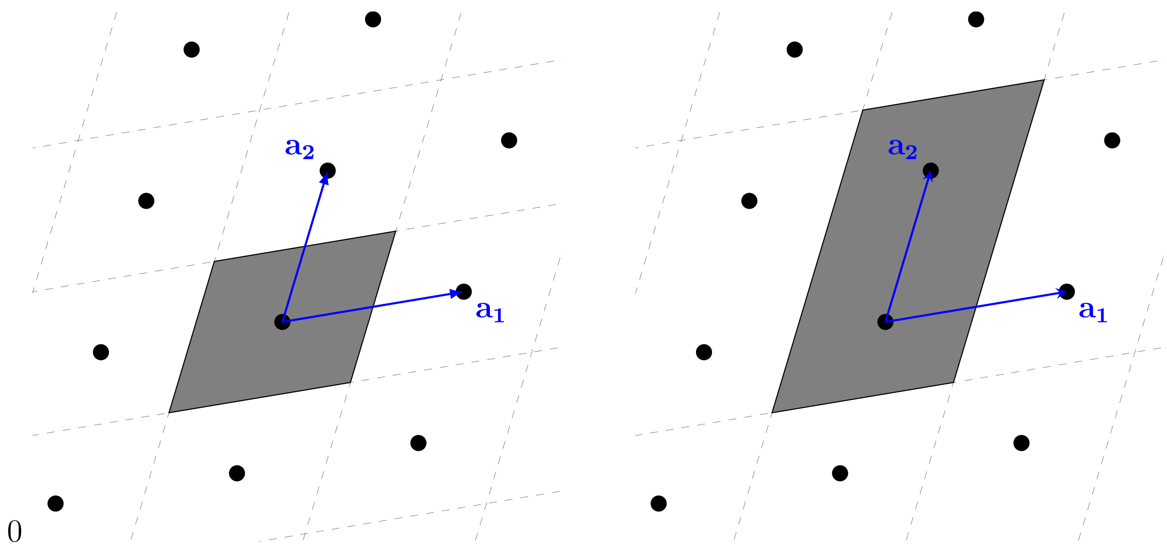


Figure 3: An example of a lattice in 2D. *Left*: The space is divided into primitive unit cells, each containing one lattice point. *Right*: The space is divided into non-primitive unit cells, each containing two lattice points.

3 Point groups

3.1 Discrete subgroups of $E(3)$

Let V be a subset of $\mathbb{R}^3$. The complete symmetry group of V is given by

$$\mathscr{S} = \{s \in E(3) \mid s \circ V = V\}.$$

It is easy to show that any subgroup of $\mathscr{S}$ is a symmetry group of V. For general V, finding all the symmetry groups is a difficult task but in our case, we only need to consider the discrete symmetry groups and restrict V to be of finite extent.

We define a **ball** of radius $r > 0$ centered at $\mathbf{y}$ by

$$B_r(\mathbf{y}) = \{\mathbf{z} \in \mathbb{R}^3 \mid \|\mathbf{z} - \mathbf{y}\| \leq r\}.$$

Then, a **discrete group** S is a subgroup of $E(3)$ such that for any $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$ and any $r > 0$, the orbit $O_{\mathbf{x}}$ under S intersects $B_r(\mathbf{y})$ at finite points. Notice that a finite subgroup of $E(3)$ is always discrete because the orbit of any point $\mathbf{x}$ can only contain finite points, but the converse is not true in general.

Let us return to the discrete symmetry groups of $V \subset \mathbb{R}^3$. We assume that V is of finite extent, i.e., we can always contain V inside some ball $B_r(\mathbf{y})$. Then, any symmetry group of V cannot contain non-trivial translation (i.e., excluding the identity), screw displacements, and glide reflections, since any composition of two symmetry transformations must still be an element of the group, but repeatedly applying one of the above transformations would move V out of $B_r(\mathbf{y})$.

One result, which we will not prove, is that if V is of finite extent, any discrete symmetry group S of V is a finite subgroup of the rotation group with respect to a fixed point $\mathbf{y}$. In section 2.2, we showed that any rotation, both proper and improper, about a fixed point is conjugate to the rotation about the origin $\mathbf{O}$, which itself is isomorphic to $O(3)$. Thus without loss of generality, we choose the fixed point to be $\mathbf{y} = \mathbf{O}$; then, determining all discrete symmetry groups is the same as finding all the finite subgroups of $O(3)$ and these are called the **point groups**. We will refer to the discrete symmetry group and the corresponding subgroup of $O(3)$ by the same letter S.

Now, define the following map to $\{1, -1\} \simeq C_2$

$$\begin{aligned} \det :\ & S \to C_2, \\ & s \mapsto \det s. \end{aligned}$$

Notice that this is a homomorphism because multiplication rule for the determinant is the same as for a group, i.e., $\det(AB) = \det(A)\det(B)$ where A, B are any two square matrices of the same size. We know that $\mathrm{Ker}(\det)$ is always a normal subgroup of S and

$$S/\mathrm{Ker}(\det) \simeq \mathrm{Ran}(\det).$$

Since $|\mathrm{Ran}(\det)|$ can only be either 1 or 2, we categorize the point groups into two types†:

- **First kind** if $\mathrm{Ran}(\det) = \{1\}$ or equivalently, $\mathrm{Ker}(\det) = S$,
- **Second kind** if $\mathrm{Ran}(\det) = \{1, -1\}$ so $\mathrm{Ker}(\det)$ is a proper normal subgroup of S.

These also imply that point groups of the first kind only contain proper rotations while those of the second kind include improper rotations as well.

Let us consider point groups of the second kind. We will denote $\mathrm{Ker}(\det) = K$. It is possible to find an element $\bar{s} \in (S \setminus K)$, then we can partition S into two cosets: K and $\overline{K}$, where $\overline{K} = \bar{s}K = K\bar{s} = S \setminus K$ (since K is normal). It is easy to see that $\det(K) = \{1\}$ and $\det(\overline{K}) = \{-1\}$, so each only contains proper rotations and improper rotations, respectively. Thus, we get $S = K \cup \overline{K}$ with $K \cap \overline{K} = \varnothing$. Denoting the inversion by I, we consider the two cases:

- Case 1: S contains inversion ($I \in S$)
  Since $\det(I) = -1$, $I \notin K$. Therefore, we can set $\bar{s} = I$ to get $S = K \cup IK$.
- Case 2: S does not contain inversion ($I \notin S$)
  We cannot identify $\overline{K}$ like in the previous case so first, set $K^+ = I\overline{K}$. Notice that

1. $\det(K^+) = \{1\}$, so K^+ corresponds to proper rotations;
2. $K \cap K^+ = \varnothing^{\dagger\dagger}$;
3. $|K| = |\overline{K}| = |K^+|$.

If we define $S^+ = K \cup K^+$ and a map

$$\begin{aligned} \phi :\ S &\to S^+, \\ s &\mapsto I^{|s|}s, \end{aligned}$$

where we denote $|s| = 0$ if $s \in K$ and $|s| = 1$ if $s \in \overline{K}$. In other words,

$$\phi(s) = \begin{cases} s & \text{if } s \in K, \\ Is & \text{if } s \in \overline{K}. \end{cases}$$

It can be seen that for any $s_1, s_2 \in S$,

$$|s_1 s_2| = |s_1| + |s_2| \bmod 2.$$

Hence, we get

$$\begin{aligned} \phi(s_1 s_2) &= I^{|s_1 s_2|} s_1 s_2 \\ &= I^{|s_1|+|s_2| \bmod 2} s_1 s_2 \\ &= I^{|s_1|} s_1 I^{|s_2|} s_2 \\ &= \phi(s_1)\phi(s_2), \end{aligned}$$

where we have used the fact that I commutes with any (3×3) matrix and $I^m = I^{2k+m}$ for $m = 0, 1$ and $k \in \mathbb{N}$. As a result, ϕ is a homomorphism and moreover, it is, in fact, an isomorphism so we can write $S \simeq S^+$.

Finite groups of proper rotations such as K and K^+ can be identified with the point groups of the first kind, so we can construct all finite point groups only by focusing on those of the first kind.

We will summarize the above result as follows: Let S be finite subgroup of $O(3)$, define $K = S \cap SO(3)$ and $\overline{K} = S \setminus K$, then there are exactly three possibilities

$$S \simeq \begin{cases} K & \text{if } \mathrm{Ran}(\det) = \{1\}, \\ K \cup IK & \text{if } \mathrm{Ran}(\det) = \{1, -1\} \text{ and } I \in S, \\ K \cup I\overline{K} & \text{if } \mathrm{Ran}(\det) = \{1, -1\} \text{ and } I \notin S, \end{cases}$$

where $\simeq$ is used to imply either an isomorphism or an equality.

†Note: It is not possible to have $\mathrm{Ran}(\det) = \{-1\}$ (or $\mathrm{Ker}(\det) = \varnothing$) because it would mean that for any $A, B \in S$, $\det(A) = \det(B) = -1$, but since $AB \in S$, we have $\det(AB) = \det(A)\det(B) = 1$ so $\mathrm{Ran}(\det)$ has to contain 1, leading to a contradiction.

††Note: For any $s \in S$, we have $Is \notin S$. This is because if the opposite was true, i.e., $Is \in S$, then we would get $Iss^{-1} = I \in S$ followed from $s^{-1} \in S$. As a result, S does not contain any element of $K^+ = I\overline{K}$ so $K \cap K^+ = \varnothing$.

3.2 Point groups of the first kind

Let us consider S to be a non-trivial finite subgroup of $SO(3)$, so S only contains proper rotations and $|S| \geq 2$. If we let S act on a ball B_r of some radius r and centered at the origin, S will map B_r onto itself. Now, we define $\mathbf{x} \in B_r$ to be a **pole** associated with $s \in S$ where $s \neq \mathbb{I}$ if $s \circ \mathbf{x} = \mathbf{x}$. Because s is a rotation, the poles of s correspond to the intersections between the axis of rotation and B_r (see Figure 4). Also, notice that if $\mathbf{x}$ is a pole associated with s and s' is another element of S, one has

$$(s'ss'^{-1}) \circ (s' \circ \mathbf{x}) = (s'ss'^{-1}s') \circ \mathbf{x} = (s's) \circ \mathbf{x} = s' \circ (s \circ \mathbf{x}) = s' \circ \mathbf{x},$$

meaning that $s' \circ \mathbf{x}$ is another pole which is associated with $s'ss'^{-1} \in S$. As a result, every element of S maps poles to poles so we can consider S as a transformation group that permutes the poles. Let us define

- The set of all poles: $X = \{\mathbf{x}_i\}_i$,
- The stabilizer of $\mathbf{x}_i$: $S_{\mathbf{x}_i}$ with $n_i = |S_{\mathbf{x}_i}|$,
- The orbit of $\mathbf{x}_i$: $O_{\mathbf{x}_i}$ with $p_i = |O_{\mathbf{x}_i}|$.

Also, we will denote $n = |S|$. Using the result from section 2.1, we have $p_i = n/n_i$ or $n_i = n/p_i$. The second equation implies that n_i is the same for any pole in the same orbit. Recall that the orbits are equivalence classes, so we can partition X into

$$X = \bigcup_{j=1}^{\mathscr{P}} O_j \quad \text{with} \quad O_j \cap O_k = \varnothing \quad \text{whenever} \quad j \neq k,$$

where $\mathscr{P}$ is the total number of orbits. Then, n_i and p_i are properties of the orbit (and not individual element) so we will refer to them by $n_j = |S_{\mathbf{x}_{i \in O_j}}|$ and $p_j = |O_j|$ instead. Excluding the trivial rotation, the total number of rotations that fix some pole in O_j is

$$\begin{aligned}
&\#\text{poles in } O_j \\
&\times \#\text{non-trivial rotations fixing some } \mathbf{x}_i \in O_j \\
&= p_j(n_j - 1) \\
&= n\left(1 - \frac{1}{n_j}\right).
\end{aligned}$$

We have $\mathscr{P}$ orbits, so the total number of non-trivial rotations fixing some pole in X is

$$n \sum_{j=1}^{\mathscr{P}} \left(1 - \frac{1}{n_j}\right).$$

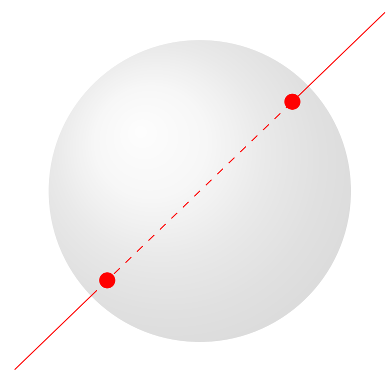


Figure 4: A rotation on the ball B_r. The line corresponds to the axis of rotation and the dots correspond to the poles.

Every rotation is associated with two poles, meaning that each distinct rotation is counted twice in the sum above. Therefore, we get

$$2(n-1) = n\sum_{j=1}^{\mathscr{P}}\left(1-\frac{1}{n_j}\right) \quad \text{or} \quad 2\left(1-\frac{1}{n}\right) = \sum_{j=1}^{\mathscr{P}}\left(1-\frac{1}{n_j}\right),$$

where the -1 is added to account for the trivial rotation.

Next, we would like to find all the possible values of $\mathscr{P}$ and $\{n_j\}_j$. Notice that $n \geq n_j \geq 2$ because n_j always includes the identity element, so we have

$$\sum_{j=1}^{\mathscr{P}}\frac{1}{n_j} \leq \frac{\mathscr{P}}{2}.$$

Then, from the previous equality,

$$2\left(1-\frac{1}{n}\right) = \sum_{j=1}^{\mathscr{P}}\left(1-\frac{1}{n_j}\right) = \mathscr{P} - \sum_{j=1}^{\mathscr{P}}\frac{1}{n_j} \geq \frac{\mathscr{P}}{2}.$$

As a result,

$$\mathscr{P} \leq 4\left(1-\frac{1}{n}\right) < 4.$$

Also, if $\mathscr{P} = 1$, we have

$$2\left(1-\frac{1}{n}\right) = 1-\frac{1}{n_1} \quad \text{or} \quad \frac{1}{n_1} = \frac{2}{n} - 1 \leq 0,$$

which is not satisfied for $n_1 \geq 2$. Thus, we end up with only two possibilities, which are either $\mathscr{P} = 2$ or $\mathscr{P} = 3$. We refer the readers to [1,2] for the calculation as we will simply state all the possible solutions to $\{n_j\}$. From there, we calculate $\{p_j\}$ using $p_i = n/n_i$, then we can find the total number of poles

$$p = \sum_j p_j,$$

as well as the number of axes of rotation

$$\#\text{AOR} = \frac{p}{2}.$$

Without loss of generality, we assume that $n_1 \leq n_2 \leq n_3$, then we have

- If $\mathscr{P} = 2$:
  + $(n_1, n_2) = (n, n)$ where $n = 2, 3, 4, \ldots$:

    This gives

$$(p_1, p_2) = (1, 1) \quad , \quad p = 2 \quad , \quad \#\text{AOR} = 1.$$

There are only two poles and an axis of rotation passing through these two poles, so we get

$$S = \{\text{Rotations about this axis by } \frac{2\pi}{n}k \text{ with } k \in \mathbb{Z}\} \simeq C_n,$$

the **cyclic group of order $\boldsymbol{n}$**. We say that an axis is **$\boldsymbol{n}$-fold** if the group of rotations about this axis is isomorphic to C_n.

– If $\mathscr{P} = 3$:

+ $(n_1, n_2, n_3) = (2, 2, m)$ and $n = 2m$ where $m = 2, 3, 4...$:

  This gives

$$(p_1, p_2, p_3) = (m, m, 2) \quad , \quad p = 2m + 2 \quad , \quad \#\text{AOR} = m + 1.$$

  These include m 2-fold axes and one m-fold axis. This is called the **dihedral group of order $\boldsymbol{2m}$**, denoted by D_m.

+ $(n_1, n_2, n_3) = (2, 3, 3)$ and $n = 12$:

  This gives

$$(p_1, p_2, p_3) = (6, 4, 4) \quad , \quad p = 14 \quad , \quad \#\text{AOR} = 7.$$

  These include four 3-fold axes and three 2-fold axes. This is called the **tetrahedral group**, denoted by T.

+ $(n_1, n_2, n_3) = (2, 3, 4)$ and $n = 24$:

  This gives

$$(p_1, p_2, p_3) = (12, 8, 6) \quad , \quad p = 26 \quad , \quad \#\text{AOR} = 13.$$

  These include three 4-fold axes, four 3-fold axes, six 3-fold axes. This is called the **octahedral group**, denoted by O.

+ $(n_1, n_2, n_3) = (2, 3, 5)$ and $n = 60$:

  This gives

$$(p_1, p_2, p_3) = (30, 20, 12) \quad , \quad p = 62 \quad , \quad \#\text{AOR} = 31.$$

  These include six 5-fold axes, ten 3-fold axes, fifteen 2-fold axes. This is called the **icosahedral group**, denoted by I.

It is also informative to know some representative shapes that exhibits these symmetries (examples are given in Figure 5)

- C_n: an n-pyramid,
- D_m: an m-prism (or a 2D m-gon in 3D),
- T: a tetrahedron,
- O: an octahedron or a cube,
- I: an icosahedron or a dodecahedron.

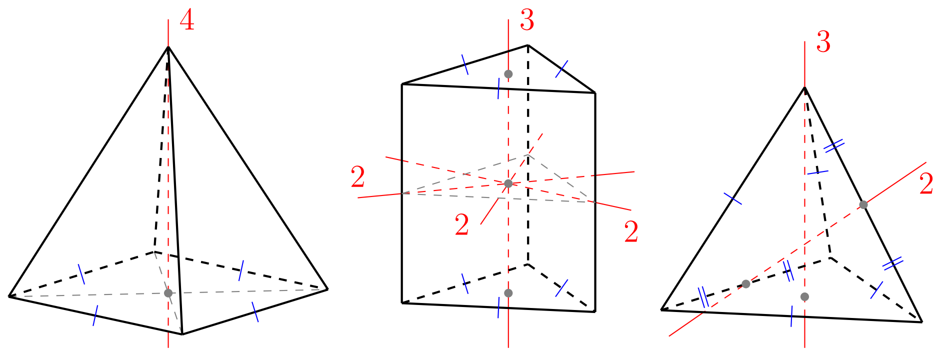


Figure 5: Examples of symmetric shapes. The red lines are the axes of rotation and the numbers are the orders of the corresponding cyclic groups. *Left*: A 4-pyramid (C_4). *Middle*: A 3-prism (D_3). *Right*: A tetrahedron (T, not all axes of rotation are drawn)

3.3 Point groups of the second kind

Using the result of section 3.1, we can construct the point groups of the second kind for two cases, either the inversion (which we will denote by $\mathbf{I}$ to differentiate it with the icosahedral group) is in S or not

- If $\mathbf{I} \in S$:

  (1) $S = C_m \cup \mathbf{I}C_m$ $(n = 2m)$

  (2) $S = D_m \cup \mathbf{I}D_m$ $(n = 4m)$

  (3) $S = T \cup \mathbf{I}T$ $(n = 24)$

  (4) $S = O \cup \mathbf{I}O$ $(n = 48)$

  (5) $S = I \cup \mathbf{I}I$ $(n = 120)$

- If $\mathbf{I} \notin S$:

  We first want to find a point group of the first kind S^+ such that it contains a subgroup K with $|S^+|/|K| = 2$, so we get $S^+ = K \cup K^+$ where K^+ is the other coset. Then, we can define a point group of the second kind $S = K \cup \mathbf{I}K^+ \simeq S^+$ which does not contain $\mathbf{I}$ because the identity element $e \notin K^+$ by virtue of the construction. All the possible cases are

(6) $K = C_m$ and $S^+ = C_{2m}$ $(n = 2m)$

(7) $K = C_m$ and $S^+ = D_m$ with $m \geq 2$ $(n = 2m)$

(8) $K = D_m$ and $S^+ = D_{2m}$ with $m \geq 2$ $(n = 4m)$

(9) $K = T$ and $S^+ = O$ $(n = 24)$

However, many of these cases can be classified into the same category. Here, we will follow the **Schönflies notation** (in fact, we have already used them in the previous section). For convenience, we will denote a rotation of $2\pi/m$ about an axis of interest by $\mathbf{R_m}$, a reflection about a plane perpendicular to that axis by $\mathbf{M_h}$ (M for mirror and h for horizontal), and a reflection about a plane containing that axis by $\mathbf{M_v}$ (v for vertical). Then, we have

+ $\begin{cases} \text{(1) for odd } m \\ \text{(6) for even } m \end{cases}$

  $\longrightarrow$ S_{2m}: a cyclic group of order $n = 2m$ generated by the rotation-reflection $\mathbf{R_{2m}M_h}$. In other words, we get

$$S_{2m} = \{(\mathbf{R_{2m}M_h})^k \mid k \in \mathbb{Z}\}.$$

  One can see that $\{(\mathbf{R_{2m}M_h})^k \mid k \in \mathbb{Z} \text{ and even}\} \simeq C_m$, so it is a subgroup of S_{2m}.

+ $\begin{cases} \text{(1) for even } m \\ \text{(6) for odd } m \end{cases}$

  $\longrightarrow$ C_{mh}: a group of order $n = 2m$ that is formed by C_m about an axis with an addition of one mirror plane corresponding to the operation $\mathbf{M_h}$, i.e.,

$$C_{mh} = \{(\mathbf{R_m})^k (\mathbf{M_h})^l \mid k, l \in \mathbb{Z}\}.$$

+ $\begin{cases} \text{(2) for even } m \\ \text{(8) for odd } m \end{cases}$

  $\longrightarrow$ D_{mh}: a group of order $n = 4m$ that is formed by D_m with an addition of $m+1$ mirror planes: one (horizontal) plane that is perpendicular to the m-fold axis and contains m 2-fold axes, and m (vertical) planes, each of which contains the m-fold axis and one of the 2-fold axes [1]. It can be seen that it has C_{mh} as a subgroup.

+ $\begin{cases} \text{(2) for odd } m \\ \text{(8) for even } m \end{cases}$

[1] The addition of the horizontal mirror plane is sufficient to define this group because the vertical mirror planes follows directly from it.

$\longrightarrow$ D_{md} (d for diagonal): a group of order $n = 4m$ that is formed by D_m with an addition of m (vertical) mirror planes, each of which contains the m-fold axis and lies between two 2-fold axes. These are also called diagonal planes. This group has S_{2m} as a subgroup.

+ (3) $\longrightarrow$ T_h: the inclusion of $\mathbf{I}$ in T results in three "horizontal" mirror planes, each of which contains two 2-fold axes.

+ (4) $\longrightarrow$ O_h: O with inversion symmetry

+ (5) $\longrightarrow$ I_h: I with inversion symmetry

+ (7) $\longrightarrow$ C_{mv}: a group of order $n = 2m$ that is formed by C_m about an axis with an addition of m (vertical) mirror planes that correspond to $\mathbf{M_v}$'s and each are rotated with respect to each other by a multiple of $2\pi/m$. Then, we have

$$C_{mv} = \{(\mathbf{R_m})^k \left(\mathbf{M_v^{(i)}}\right)^l \mid i = 1, 2, \cdots, m; k, l \in \mathbb{Z}\}.$$

+ (9) $\longrightarrow$ T_d: T with six "diagonal" mirror planes, each contains one 2-fold axis and lies between the other two 2-fold axes.

These are all the possible point groups of the second kind [2].

To summarize, the point groups of the first kind are

$$C_1 \text{ (trivial)}, C_2 = D_1, C_{m>2}, D_{m\geq 2}, T, O, I,$$

and point groups of the second kind are

$$S_2 = \{e, \mathbf{I}\}, C_{1h} = C_{1v} = \{e, \mathbf{M}\}, C_{2h} = D_{1d}, C_{2v} = D_{1h}, S_{2(m\geq 2)}, C_{(m>2)h}, C_{(m>2)v},$$

$$D_{(m\geq 2)h}, D_{(m\geq 2)d}, T_h, T_d, O_h, I_h.$$

Another way to classify these symmetry groups is by the **Hermann–Mauguin notation**, which regards improper rotations in terms of *rotoinversion* (a rotation about an axis with an inversion about a point on that axis) instead of *rotoreflection* (a rotation about an axis with a reflection about a plane perpendicular to that axis) like in the case of the Schönflies notation. Readers can refer to [4] for the definition and the conversion table between the two notations.

4 Crystallographic point group

Recall that we defined a lattice by the set

$$L = \{\mathbf{l} \in \mathbb{R}^3 \mid \mathbf{l} = m_1\mathbf{a_1} + m_2\mathbf{a_2} + m_3\mathbf{a_3}, m_i \in \mathbb{Z}\}.$$

[2] We should not think too much about the number of mirror planes because there are cases when they coincide with each other. It is, instead, better to just know how these planes are constructed.

Then, a **crystallographic point group** of L is a (finite) subgroup of $E(3)$ that leaves L invariant and fixes a point $\mathbf{l_0} \in L$. The largest crystallographic point group of L at $\mathbf{l_0}$ is called the **holohedry** of L at $\mathbf{l_0}$. Since the lattice is periodic, we can equivalently work in the special case where $\mathbf{l_0} = \mathbf{O}$ alone. It is easy to see that a crystallographic point group has to be a point group itself (as defined in the previous sections).

The periodicity of the lattice also put a restriction on the type of rotational symmetry that we can have. Let S be a crystallographic point group of L and consider $R_{m,\pm} \in S$ to be a rotation of $2\pi/m$ about some axis, either without (denoted by $+$) or with (denoted by $-$) a reflection about the plane perpendicular to that axis. Then for some $\mathbf{l} \in L$, i.e.,

$$\mathbf{l} = m_1\mathbf{a_1} + m_2\mathbf{a_2} + m_3\mathbf{a_3},$$

with $m_i \in \mathbb{Z}$, we must have $R_{m,\pm} \circ \mathbf{l} \in L$. This means that there exists n_i's such that $n_i \in \mathbb{Z}$ and

$$R_{m,\pm} \circ \mathbf{l} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}.$$

In the $\mathbf{a_i}$'s basis, we can write $R_{m,\pm}$ as a 3×3 matrix which we will denote by $R^{(\mathbf{a})}_{m,\pm}$. The above equation then reads

$$(R_{m,\pm} \circ \mathbf{l})_i = (R^{(\mathbf{a})}_{m,\pm}\mathbf{l})_i = \sum_{j=1}^{3} (R^{(\mathbf{a})}_{m,\pm})_{ij} m_j = n_i.$$

For some k, let $m_j = \delta_{jk}$ for all j where δ_{jk} is the Kronecker delta, so $\mathbf{l} = \mathbf{a_k}$. Then, we have

$$\sum_{j=1}^{3} (R^{(\mathbf{a})}_{m,\pm})_{ij}\delta_{jk} = (R^{(\mathbf{a})}_{m,\pm})_{ik} = n_i \in \mathbb{Z}.$$

which has to be true for any choice of i, k. Thus, we arrive at the result that $(R^{(\mathbf{a})}_{m,\pm})_{ik} \in \mathbb{Z}$ for any i, k. Assume that we want to work with a different basis $\mathbf{b_i}$'s of $\mathbb{R}^3$, then we have the matrix of $R_{m,\pm}$ in this basis denoted by $R^{(\mathbf{b})}_{m,\pm}$ with the relation

$$R^{(\mathbf{b})}_{m,\pm} = MR^{(\mathbf{a})}_{m,\pm}M^{-1}$$

where M is the change of basis matrix. Taking the trace of this relation gives us

$$\mathrm{Tr}(R^{(\mathbf{b})}_{m,\pm}) = \mathrm{Tr}(MR^{(\mathbf{a})}_{m,\pm}M^{-1}) = \mathrm{Tr}(M^{-1}MR^{(\mathbf{a})}_{m,\pm}) = \mathrm{Tr}(R^{(\mathbf{a})}_{m,\pm}),$$

where we have used the cyclic property of the trace. Since we have shown that all elements of $R^{(\mathbf{a})}_{m,\pm}$ are integers, we find that for any choice of basis $\mathbf{b_i}$'s, we have

$$\mathrm{Tr}(R^{(\mathbf{b})}_{m,\pm}) \in \mathbb{Z}.$$

Recall that a rotation of ϕ about the z-axis and a reflection about the xy-plane can be represented in matrix form as

$$R(\phi\hat{\mathbf{z}}) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad M_{xy} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

in the standard basis. We can choose $\mathbf{b_i}$ such that they are orthonormal, so we can denote them to be the same as the standard basis. Letting the z-axis to be oriented in the same direction as the axis of rotation gives us

$$\mathrm{Tr}(R^{(\mathbf{b})}_{m,\pm}) = \mathrm{Tr}\begin{pmatrix}\cos(2\pi/m) & -\sin(2\pi/m) & 0\\ \sin(2\pi/m) & \cos(2\pi/m) & 0\\ 0 & 0 & \pm 1\end{pmatrix} = 2\cos\left(\frac{2\pi}{m}\right) \pm 1 \in \mathbb{Z}.$$

Using the fact that $|\cos\phi\,| \leq 1$, the above relation is equivalent to saying that

$$\cos\left(\frac{2\pi}{m}\right) \in \left\{0, \pm\frac{1}{2}, \pm 1\right\}.$$

Here, we focus on the generator of rotation about an axis, i.e., we only consider $m = 1, 2, 3, \ldots$ Then, solving this equation gives

$$m \in \{1, 2, 3, 4, 6\}.$$

In other words, only 1-fold, 2-fold, 3-fold, 4-fold, 6-fold rotations and rotoreflections are allowed in crystallographic point groups.

With this restriction, we have 11 point groups of the first kind

$$C_1, C_2 = D_1, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T, O,$$

and 21 point groups of the second kind

$$S_2, S_4, S_6, C_{1h} = C_{1v}, C_{2h} = D_{1d}, C_{3h}, C_{4h}, C_{6h}, C_{2v} = D_{1h}, C_{3v}, C_{4v}, C_{6v},$$

$$D_{2h}, D_{3h}, D_{4h}, D_{6h}, D_{2d}, D_{3d}, T_h, T_d, O_h,$$

that can be crystallographic point groups, giving us 32 groups in total. The point groups I (as well as I_h), D_{4d}, and D_{6d} are excluded because they contain 5-fold rotation, 8-fold rotoreflection, and 12-fold rotoreflection, respectively.

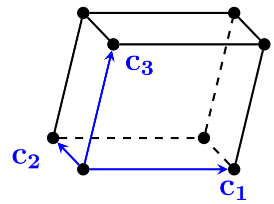
By working about the origin alone, we can speak about the holohedries of two lattices without referring to different points of reference. Then, we say that two lattices are in the same **lattice system** if they have the same holohedry. Let H be a holohedry of some arbitrary lattice L. We notice that for any $\mathbf{l} \in L$, we have $\mathbf{I} \circ \mathbf{l} = -\mathbf{l} \in L$, meaning that $\mathbf{I} \circ L = L$. Therefore, it is necessary that H is a point group of the second kind with $\mathbf{I} \in H$. Moreover, for a lattice, a C_m rotational symmetry about an axis (passing through $\mathbf{O}$) where $m = 3, 4, 6$ also gives rise to a C_{mv} symmetry about that axis. This statement can be proven by considering the transformation of the points as well as their projections on a plane perpendicular to the axis of rotation (see page 41, [2]). Then, we find the 7 holohedries (with their relations to each other) to be

$$\begin{array}{ccccccccc} S_2 & \subset & C_{2h} & \subset & D_{2h} & \subset & D_{4h} & \subset & O_h \\ & & \cap & & \cap & & & & \\ & & D_{3d} & \subset & D_{6h} & & & & \end{array}$$

These lattice systems can be further divided into 14 lattice types called the **Bravais lattices**. Let us list these lattice types along with their respective unit cells (not necessarily primitive). For convenience, we will denote the vectors that form these unit cells by $\mathbf{c_i}$'s[3], the angle between $\mathbf{c_i}$ and $\mathbf{c_j}$ by θ_{ij}.

– **Triclinic** S_2: (This also includes C_1)

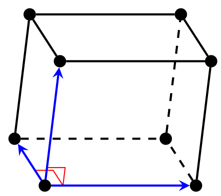
  $\mathbf{c_i}$'s can be arbitrary. We only have the primitive type.



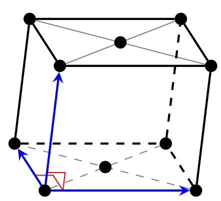
– **Monoclinic** C_{2h}: (This also includes C_2, C_{1h})

  $\theta_{12} = \theta_{13} = 90°$. We have two types:

  + Primitive:



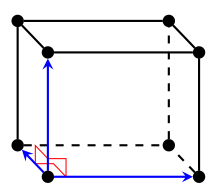
  + Base-centered:



– **Orthorhombic** D_{2h}: (This also includes D_2, C_{2v})

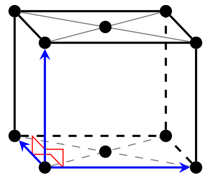
  $\theta_{12} = \theta_{23} = \theta_{13} = 90°$. We have four types:

  + Primitive:

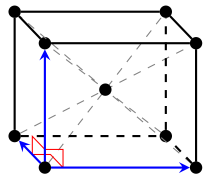


[3]Generally, these are not the primitive basis vectors.

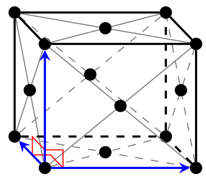
+ Base-centered:



+ Body-centered:



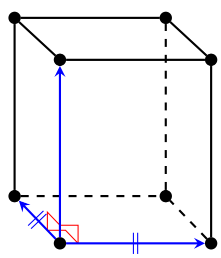
+ Face-centered:



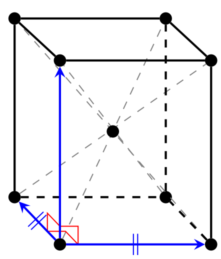
– **Tetragonal** D_{4h}: (This also includes $C_4, D_4, S_4, C_{4h}, C_{4v}, D_{2d}$)

$|\mathbf{c_1}| = |\mathbf{c_2}|$ and $\theta_{12} = \theta_{23} = \theta_{13} = 90°$. We have two types:

+ Primitive:

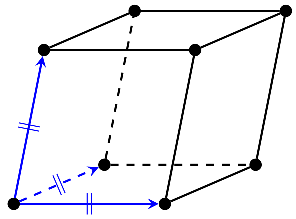


+ Body-centered:



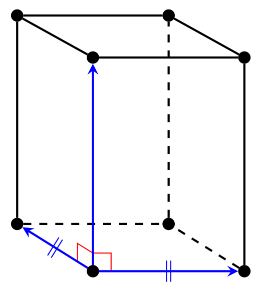
– **Rhombohedral** D_{3d}: (This also includes C_3, D_3, S_6, C_{3v})

$|\mathbf{c_1}| = |\mathbf{c_2}| = |\mathbf{c_3}|$ and $\theta_{12} = \theta_{23} = \theta_{13}$. We only have the primitive type.



– **Hexagonal** D_{6h}: (This also includes $C_6, D_6, C_{3h}, C_{6h}, C_{6v}, D_{3h}$)

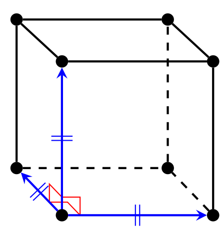
$|\mathbf{c_1}| = |\mathbf{c_2}|$, $\theta_{13} = \theta_{23} = 90°$, and $\theta_{13} = 120°$. We only have the primitive type.



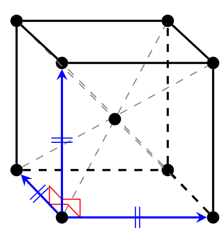
– **Cubic** O_h: (This also includes T, O, T_h, T_d)

$|\mathbf{c_1}| = |\mathbf{c_2}| = |\mathbf{c_3}|$ and $\theta_{12} = \theta_{23} = \theta_{13} = 90°$. We have three types:

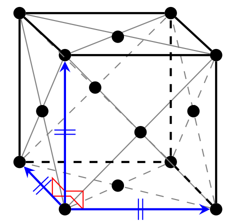
+ Primitive:



+ Body-centered:



+ Face-centered:



This concludes our analysis of crystallographic point groups. We have not taken into account the translational symmetry of a lattice which, together with the crystallographic point groups, forms the **crystallographic space groups** or just **space groups**. In total, there are 230 space groups. We refer the readers to [6] for more information on this subject.

5 References

[1] Groups and Their Representations, lecture notes (old and new) by S. Richard.
[2] Symmetry Groups and Their Applications, textbook by W. Miller.
[3] Schönflies notation (Wikipedia).
[4] Hermann-Mauguin notation (Wikipedia).
[5] Crystal system (Wikipedia).
[6] Space group (Wikipedia).