Why is it Important?

We can classify molecules (biocomplexes) according to the level of their symmetry elements, so they can be grouped together having the same set of symmetry elements.

This classification is very important, because it allows to make some general conclusions about molecular properties without extra calculation. On the atomic level it helps to reveal the molecular properties without any calculations.

On atomic level, we will be able to decide if a molecule has a dipole moment or not, and to know how these property are reflected on their surfaces.

What sort of interaction hold biomolecules together in huge biocomplexes such as viruses, secretion systems, etc.
We say that such an object is symmetric with respect to a given operation if this operation, when applied to the object, does not appear to change it.

Symmetry may depend on the properties under consideration:

- **for an image** we may consider just the shapes, or also the colors;
- **for an object (3D)**, we may additionally consider density, chemical composition, contacts between domains, etc.

**Biological objects**

The person - hereafter referred to as ‘it’ has a mirror plane, provided it stands straight (and that we ignore its internal organs). Each half of the figure is an asymmetric unit.

Moving an arm or leg destroys the symmetry and the whole figure can then be treated as an asymmetric unit. This little ‘object’, both with and without its mirror plane will be used to illustrate further symmetry elements, and to build more complicated groups.

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**Operations with Multimeric Functions**

1D \(\rightarrow\) 2D \(\rightarrow\) 3D

There are two types operations with functions in one-dimensional space.

1. **Translation**
   \[ g(x) = g(x + a) \]
Operations with Multimeric Functions

2. Reflection (mirror) \( g(x) = g(b - x) \)

These operations can be combined

\[ g_1(x) = g_1(x + a) = g(x + a) + g(b - a - x) \]

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Operations with Multimeric Functions

1D → 2D → 3D

There are three types operations with images **in plane:**

1. Translation in two directions
2. Reflection
3. Rotation **in plane**

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Operations with Multimeric Functions

**Translation** in ONE direction

\[ g(\vec{r}) = g(\vec{r} + \vec{a}) \]

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Operations with Multimeric Functions

**Translation** in two directions

\[ g(\vec{r}) = g(\vec{r} + k\vec{a} + l\vec{b}) \]
Reflection = mirror  \[ g(\vec{r}) = g(\vec{a} - \vec{r}) \]

There is a plain between objects. So the distance from any point of the object and the plain is the same as the distance between the same point of the mirrored object and the plain.

Mirror-image symmetry

This is the most familiar and conventionally taught type of symmetry. It applies for instance for the letter \( T \): when this letter is reflected along a vertical axis, it appears the same. \( T \) has a vertical symmetry axis.

A reflection "flips" an object over a line (in 2D) or plane (in 3D), inverting it to its mirror image, as if in a mirror. If the result is the same then we have mirror-image symmetry (also known in the terminology of modern physics as P-symmetry).

Operations with Multimeric Functions

Translation

Operations with Multimeric Functions

Rotation in plane

73°
Inversion $g(r) = g(-r)$

There is a point between objects. So the distances from any point of the object and the point are the same as the distances between the similar points of the inversed object and the point.

Rotational symmetry $C_n$

A rotation rotates an object about a point (in 3D: about an axis). Rotational symmetry of order $n$, also called $n$-fold rotational symmetry, with respect to a particular point or axis means that rotation by an angle of $360^\circ/n$ does not change the object.

\[
(180^\circ, 120^\circ, 90^\circ, 72^\circ, 60^\circ, 51.43^\circ, 45^\circ, 40^\circ, \ldots, 2, 3, 4, 5, 6, 7, 8, 9, \text{ etc})
\]

For each point or axis of symmetry the symmetry group is isometric with the cyclic group $C_n$ of order $n$. The fundamental domain is a sector of $360^\circ/n$.

\[
C_2, C_3, C_4, C_5, C_6, C_7, C_8, C_9, \ldots
\]

One point remains unmoved, which is the rotation point.

Symmetry combinations

More complex symmetries are combinations of reflectional, rotational, translational, and glide reflection symmetry.

Mirror-image symmetry in combination with $n$-fold rotational symmetry, with the point of symmetry on the line of symmetry, implies mirror-image symmetry with respect to lines of reflection rotated by multiples of $180^\circ/n$, i.e. $n$ reflection lines which are radially spaced evenly (for odd $n$ this already follows from applying the rotational symmetry to a single reflection axis, but it also holds for even $n$).
The five basic lattice types

There are 17 space groups in the plane, but their unit cells fall into one of five basic shapes as follows: repeating patterns in the plane can only have 1, 2, 3, 4 or 6-fold symmetry. In particular, repeating patterns in the plane cannot have five-fold symmetry.

What is about five-fold symmetry? The element of the unit cell may have 5-fold symmetry but the overall symmetry of the pattern does not. In recent years some materials have turned up with five-fold symmetry. These materials, termed quasicrystals, do not have repeating patterns.

http://www.spsu.edu/math/tile/symm/ident17.htm
Combination of symmetries in plane

Proteins don’t do this – pack by translations

Symmetry in 3D space

Three types operations with objects in space

Translation in three directions
Reflection (mirror) in space
Rotation (Inversion)

Rotations can be combined with translations and reflections, however they cannot be combined in an arbitrary way. Symmetry operators impose constrains.

Combination of operators can generate infinite lattices as we can see that in crystals.
Symmetry in 3D space

A space relationship between elements in each oligomeric molecule can be described by a set of symmetry operations that describes the overall molecular symmetry. This combination of operations define the **POINT GROUP** of the molecule.

One point remains unchanged.
There are no translational operators.
Combination of rotation, mirror and inversion gives 32 combinations.
But for the proteins we will have only 11 combinations: no inversion or mirror.
Symmetry in 3D space

In three dimensions we can distinguish **cylindrical symmetry** and **spherical symmetry** (no change when rotating about one axis, or for any rotation).

There is no dependence on the angle using cylindrical coordinates and no dependence on either angle using spherical coordinates. Cylindrical symmetry is very often called as cyclical symmetry.

The simplest symmetry is **C1**, if the object does not have any symmetry at all.

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Basic symmetry operations in space

- **Cn** (for cyclic) indicates that the group has an \( n \)-fold rotation axis.
- **Sn** (for Spiegel, German for mirror) denotes a group that contains only an \( n \)-fold rotation-reflection axis.
- **D** (for dihedral, or two-sided) indicates that the group has an \( n \)-fold rotation axis plus a two-fold axis perpendicular to that axis.

In crystallography this applies only for \( n = 1, 2, 3, 4, 6 \), due to the **crystallographic restriction theorem**.

http://csi.chemie.tu-darmstadt.de/ak/immel/tutorials/symmetry/index4.html
Symmetry in 3D space

Rotational symmetry is Cn, if the object has several elements, that arranged in a circular system. The number of elements determines the order of symmetry.

Symmetry C2

Projections

Symmetry C3

Projections of the object rotational symmetry and their symmetry.

Symmetry C4

Rotational symmetry

Ca release channel 2.4 Mda
a-Latrotoxin 520kDa
C13

Symmetry C5

Portal protein SPP1

Symmetry D2

Ca release channel 2.4 Mda
a-Latrotoxin 520kDa
C13
Symmetry in 3D space

Dihedral point group symmetry Dn are a combination of cyclical symmetries with a two-fold axis, which is perpendicular to the axis of rotation. 

Palinurus elephas hemocyanin (75kDa x 6)

Keyhole Limpet Hemocyanin

Symmetry in 3D space

Dihedral point group symmetry Dn are a combination of cyclical symmetries with a two-fold axis, which is perpendicular to the axis of rotation.

222 D2

D3

32 D3

D5

52 D5

Platonic and Archimedean Polyhedra

The Platonic Solids, discovered by the Pythagoreans but described by Plato (in the Timaeus) and used by him for his theory of the 4 elements, consist of surfaces of a single kind of regular polygon, with identical vertices.

The Archimedean Solids, consist of surfaces of more than a single kind of regular polygon, with identical vertices and identical arrangements of polygons around each polygon.

Cubic pointgroup symmetries

T - 23 Tetrahedral symmetry requires a minimum of 12 identical subunits
O - 432 Octahedral point group symmetry, needs 24 subunits
I - 532 Icosahedral symmetry, 60 subunits
Cube

Octahedron

Combination of symmetries in 3D

Dodecahedron

Icosahedron
Combination of symmetries in 3D

http://www.staff.ncl.ac.uk/j.p.goss/symmetry/

Icosahedrael symmetry

The high-symmetry point groups in which more than one \( C_n \) axis with \( n \geq 3 \) is present are best visualized by the five regular polyhedra (Platonic solids) as shown below. In these objects, all faces, vertices, and edges are symmetry related and thus equivalent. The octahedron and the cube are close related to each other as they contain the same symmetry elements, but in different orientations. The same applies to the dodecahedron and icosahedron.

<table>
<thead>
<tr>
<th>Graphics</th>
<th>Tetrahedron</th>
<th>Octahedron</th>
<th>Cube</th>
<th>Dodecahedron</th>
<th>Icosahedron</th>
</tr>
</thead>
<tbody>
<tr>
<td>Faces</td>
<td>4 triangles</td>
<td>8 triangles</td>
<td>6 squares</td>
<td>12 pentagons</td>
<td>20 triangles</td>
</tr>
<tr>
<td>Vertices</td>
<td>4</td>
<td>6</td>
<td>8</td>
<td>20</td>
<td>12</td>
</tr>
<tr>
<td>Edges</td>
<td>6</td>
<td>12</td>
<td>12</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>Point Group</td>
<td>( T_d )</td>
<td>( O_h )</td>
<td>( O_h )</td>
<td>( I_h )</td>
<td>( I_h )</td>
</tr>
</tbody>
</table>

For each of the point groups \( T_d, O_h, \) and \( I_h \) there exists sub-groups \( T, O, \) and \( I \) which contain all \( C_n \) symmetry elements, but none of the \( S_n \) operations (including inversion and reflection). Adding a \( \sigma_h \) mirror plane or an inversion center to the \( T \) group yields \( T_d \).
Further reading


Schoenflies notation

In Schoenflies notation, point groups are denoted by a letter symbol with a subscript. The symbols mean the following:

The letter **I** (for icosahedron) indicates that the group has the symmetry of an icosahedron.

The letter **O** (for octahedron) indicates that the group has the symmetry of an octahedron (or cube).

The letter **T** (for tetrahedron) indicates that the group has the symmetry of a tetrahedron.

1. Look at the molecule and see if it seems to be very symmetric or very unsymmetric. If so, it probably belongs to one of the special groups (low symmetry: C₁, Cₐ, Cₐ or linear, Cᵥ, Dᵥ) or high symmetry (T_d, O_h, I_h).

2. For all other molecules find the rotation axis with the highest n, the highest order Cₙ axis of the molecule.

3. Does the molecule have any C₂ axes perpendicular to the Cₙ axis? If it does, there will be n of such C₂ axes, and the molecule is in one of D point groups. If not, it will be in one of C or S point groups.

4. Does it have any mirror plane (sᵥ) perpendicular to the Cₙ axis. If so, it is Cᵥₙ or Dᵥₙ.

5. Does it have any mirror plane (s_d)? If so, it is Cᵥₙ or Dᵥₙ.