3.6: Representations

A **representation** is any mathematical construct that will reproduce the group multiplication table. In general, there are an infinite number of representations possible for a given group, however, most of them will be related through simple relationships, and thus can be constructed from (or reduced to) other representations. Those that cannot be reduced to linear combinations of other representations are called **irreducible representations**. The irreducible representations are particularly useful as they can be used to predict the mathematical properties of any function that is an eigenfunction of all of the symmetry elements of a group. The number of classes of operations always gives the number of irreducible representations. Each irreducible representation can be labeled as Γ_i.

To construct a representation for a group, one must assign each operation a mathematical element. For the C_{2v} point group, we can get away with using either 1 or –1 for each element. (This is a consequence of each operation belonging to its own class.) The simplest representation can be constructed by assigning each symmetry element as 1. The group multiplication table will hold, as can be seen below.

C_{2v}	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

Note that each product gives a value that corresponds to the correct element. For example, we let C_2 = 1 and σ_v = 1. The product of C_2 *σ_v yields σ_v'. And since the value we assigned σ_v'= 1 . . and $1 * 1 = 1$ . . everything worked. This particular representation seems pretty trivial since it has to work for any multiplication table that can ever be written! In fact, every point group has this type of representation. Since 1 gives all of the elements of this representation, this is called the **totally symmetric representation**.

Another representation (Γ_2) can be constructed in which E and C_2 are represented by a 1 and σ_v and $\sigma_v'$are represented by –1. In this case, the multiplication table looks as follows:

C_{2v}	1	1	-1	-1
1	1	1	-1	-1
1	1	1	-1	-1
-1	-1	-1	1	1
-1	-1	-1	1	1

It should be clear again (or easily enough verified) that this has the same pattern as the group multiplication table.

Two other representations can be constructed in this manner (with all of the elements given as either 1 or –1). Together with the first representation, these can be summarized as in the following table.

C_{2v}		E	C_2	σ_v	σ_v'
Γ_1	A_1	1	1	1	1
Γ_2	A_2	1	1	-1	-1
Γ_3	B_1	1	-1	1	-1
Γ_4	B_2	1	-1	-1	1

These irreducible representations (Γ_i) go by a standardized set of naming rules. First, the irreducible representations are all singly degenerate (no two-by-two or three-by-three matrices were needed for the representations) so all of the irreducible representations are given the symbol A or B. A is used if the representation is symmetric (1) with respect to the principle rotation axis (C_2) and B if it is antisymmetric (-1) with respect to the principle axis. The subscript is 1 if the representation is symmetric with respect to the σ_v reflection plane, and 2 if the representation is antisymmetric with respect to this plane of reflection. If an irreducible representation requires a set of two-by-two matrices, the representation is designated E, and three-by-three matrix irreducible representations are labeled T.

We'll discuss more on the difference between a reducible and irreducible representation later. First, lets work through a slightly more difficult point group. The C_{3v} point group is not abelian and requires matrices for some of the irreducible representations.

The Symmetry of a Triangular Pyramid: a more complex point group

An example of a point group that requires two-by-two matrix elements for the irreducible representations is the C_{3v} point group. This point group (which describes the symmetry elements of an ammonia molecule or a pyramid with an equilateral triangular base) consists of the symmetry elements E, C_3, C_3' (or C_3^2), σ_v, $\sigma_v'$and σ_v''.

In the figure to the left, the C_3 axis runs perpendicular to the base of the pyramid (you are looking straight down on the top of the pyramid) and the C_3 operation might correspond to a clockwise rotation of the figure about that axis. The C_3' axis is the same as the C_3 axis, but the C_3' operation corresponds to a *counter*clockwise rotation by $2\pi/3$ radians. Note that this operation is equivalent to performing the C_3 operation twice (hence the alternative notation of C_3^2.) The σ_v, $\sigma_v'$and σ_v'' elements are reflection planes that lie perpendicular to the base, but each containing one edge of the pyramid. The reader is left to imagine the identity element.

If the corners of the base of the pyramid are labeled for convenience, the effect of each symmetry operation can be represented as follows.

$$E*(1,2,3)=(1,2,3) \qquad \sigma_v*(1,2,3)=(1,3,2)$$
$$C_3*(1,2,3)=(3,1,2) \qquad \sigma_v'*(1,2,3)=(3,2,1)$$
$$C_3^2*(1,2,3)=(2,3,1) \qquad \sigma_v”*(1,2,3)=(2,1,3)$$

Following these permutations, it is possible to construct the group multiplication table. The group multiplication table for this group (C_{3v}) looks as follows:

$\boldsymbol{C_{3v}}$	**E**	$\boldsymbol{C_3}$	$\boldsymbol{C_3^2}$	$\boldsymbol{\sigma_v}$	$\boldsymbol{\sigma_v'}$	$\boldsymbol{\sigma_v''}$
E	E	C_3	C_3^2	σ_v	$\boldsymbol{\sigma_v'}$	σ_v''
$\boldsymbol{C_3}$	C_3	C_3^2	E	σ_v''	σ_v	$\boldsymbol{\sigma_v'}$
$\boldsymbol{C_3^2}$	C_3^2	E	C_3	$\boldsymbol{\sigma_v'}$	σ_v''	σ_v
$\boldsymbol{\sigma_v}$	σ_v	$\boldsymbol{\sigma_v'}$	σ_v''	E	C_3	C_3^2
$\boldsymbol{\sigma_v'}$	$\boldsymbol{\sigma_v'}$	σ_v''	σ_v	C_3^2	E	C_3
$\boldsymbol{\sigma_v''}$	σ_v''	σ_v	$\boldsymbol{\sigma_v'}$	C_3	C_3^2	E

From this information, it is possible to separate the operations into classes. Note, for example that $(\sigma_v)^{-1}=\sigma_v$ and $(\sigma_v')^{-1}=\sigma_v'$ and $(\sigma_v'')^{-1}=\sigma_v''$. Using these relationships, the similarity transforms of C_3 involving these operations all yield C_3^2.

$$(\sigma_v)^{-1}*C_3*\sigma_v=(\sigma_v*C_3)*\sigma_v=\sigma_v''*\sigma_v=C_3^2$$
$$(\sigma_v')^{-1}*C_3*\sigma_v'=(\sigma_v'*C_3)*\sigma_v'=\sigma_v*\sigma_v'=C_3^2$$
$$(\sigma_v'')^{-1}*C_3*\sigma_v''=(\sigma_v''*C_3)*\sigma_v''=\sigma_v'*\sigma_v''=C_3^2$$

Similarly, the similarity transforms on C_3^2 using these operations all yield C_3.

$$(\sigma_v)^{-1}*C_3^2*\sigma_v=(\sigma_v*C_3^2)*\sigma_v=\sigma_v'*\sigma_v=C_3$$
$$(\sigma_v')^{-1}*C_3^2*\sigma_v'=(\sigma_v'*C_3^2)*\sigma_v'=\sigma_v''*\sigma_v'=C_3$$
$$(\sigma_v'')^{-1}*C_3^2*\sigma_v''=(\sigma_v''*C_3^2)*\sigma_v''=\sigma_v*\sigma_v''=C_3$$

This is sufficient to indicate that the operations C_3 and C_3^2 belong to the same class. However, to show that these are the only two operations in this class. Consider the similarity transforms based on the operators E, C_3 and C_3^2 on C_3 :

$$(E)^{-1} * C_3 * E = (E * C_3) * E = E * C_3 = C_3$$
$$(C_3)^{-1} * C_3 * C_3 = (C_3^2 * C_3) * C_3 = E * C_3 = C_3$$
$$(C_3^2)^{-1} * C_3 * C_3^2 = (C_3 * C_3) * C_3^2 = C_3^2 * C_3^2 = C_3$$

The fact that the result of a similarity transform on either C_3 or C_3^2 never results in σ_v, σ_v'or σ_v'', is a consequence of the proper rotation operations belonging to a different class than the reflection planes. In fact, there are three classes of operations for this point group. This implies that there are three irreducible representations for this point group.

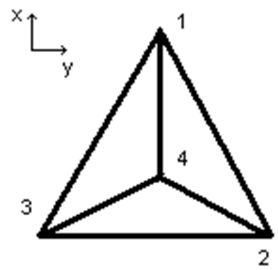

Figure 3.6.1

Another useful approach is to use matrix operators to affect the changes to the object caused by the symmetry operation. The choice of matrix operators depends on the basis set of functions being used to model the system. In this case, we will use position vectors of the corners of the bas of the pyramid. Other choices of basis might be the atomic orbitals on the atoms in a molecule. This is a very convenient choice when the task of constructing symmetry-adapted linear combinations of atomic orbitals for the purpose of modeling molecular orbitals. But I digress . . .

Consider the position vectors of the corners of the base of our trigonal pyramid. They can be specified by indicating the (x, y, z) coordinates if the origin is located in the plane of the base along the axis where all of the symmetry elements intersect.

Corner	**x**	**y**	**z**
1	0	$\frac{1}{\sqrt{3}}$	0
2	1/2	$-\frac{1}{2\sqrt{3}}$	0
3	-1/2	$-\frac{1}{2\sqrt{3}}$	0
4	0	0	h

Only corners 1, 2 and 3 will be important since none of the symmetry elements moves the fourth corner! Assuming unit length for the base edges and a height of h for the pyramid, the following table gives the (x, y, z) coordinates for each of the four corners.

From the previous discussion, we have already determined the effects of each of the symmetry operations.

$$E * (1,2,3) = (1,2,3) \qquad \sigma_v * (1,2,3) = (1,3,2)$$
$$C_3 * (1,2,3) = (3,1,2) \qquad \sigma_v' * (1,2,3) = (3,2,1)$$
$$C_3^2 * (1,2,3) = (2,3,1) \qquad \sigma_v'' * (1,2,3) = (2,1,3)$$

The task now is to construct matrix representations for each of the symmetry operations that will affect the above stated changes when matrix multiplication is used as the operation.

The identity element is easy. It will be the 3x3 identity matrix given by

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

This is easily confirmed since

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

for any choice of x, y and z. The other operations are a little trickier, but not too hard. It can be shown that the matrix that affects a rotation of α radians about the z-axis is given by

$$\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

So that the resultant of this operation is given by

$$\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x\cos\alpha - y\sin\alpha \\ x\sin\alpha + y\cos\alpha \\ z \end{pmatrix}$$

For a rotation of $2\pi/3$ radians, it is useful to note the following.

$$\cos(2\pi/3) = -1/2$$

$$\sin(2\pi/3) = \sqrt{3}/2$$

So the transformation of corner 1 of the pyramid is accomplished as follows for the C_3 operation.

$$\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1/\sqrt{3} \\ 0 \end{pmatrix} = \begin{pmatrix} -1/2 \\ -1/2\sqrt{3} \\ 0 \end{pmatrix}$$

The operation has transformed corner 1 into corner 3. It is also easily shown that the operator matrix also transforms corner 2 into corner 1, and corner 3 into corner 2. This is just as expected according to the expression shown above:

$$C_3 * (1,2,3) = (3,1,2)$$

Additionally, the matrix must satisfy the multiplication table relationship of $C_3 * C_3 = C_3^2$.

$$\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

This is the rotation matrix for a rotation of $-2\pi/3$ radians. Hence, the product worked out as expected since the C_3^2 operation is equivalent to the rotation of $-2\pi/3$ radians.

The matrix representations for the σ_v planes can be worked out by one of two methods. One is to set up the matrix equation for how a point is transformed. The other is by using the group multiplication table to generate a matrix as the product of two other operations in the group for which the matrix has already been established.

To demonstrate these methods, recall from above that the σ_v operation exchanges corners 2 and 3. The matrix for this operation must satisfy the following expression:

$$\begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \begin{pmatrix} 1/2 \\ -1/2\sqrt{3} \\ 0 \end{pmatrix} = \begin{pmatrix} -1/2 \\ -1/2\sqrt{3} \\ 0 \end{pmatrix}$$

The matrix that will affect this transformation is:

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Now, using the group multiplication table, we can generate $\sigma_v'$and σ_v'' by the relationships

$$\sigma_v * C_3^2 = \sigma_v'$$

$$\sigma_v * C_3 = \sigma_v''$$

or

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \sigma_v'$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \sigma_v\text{”}$$

The set of matrices can now be used as a representation of the group. However, these matrices can be seen as a reproducible representation of the group since they are in block-diagonal form.

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} C_3 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} C_3^2 = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\sigma_v = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \sigma_v' = \begin{pmatrix} 1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \sigma_v\text{”} = \begin{pmatrix} 1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

This representation can be broken down into two simpler representations. The first consists only of the lower right block of each of the matrices above. This yields the totally symmetric representation. The other is a representation of 2x2 matrices that are made from the upper left block of each of the matrices above. There is one other irreducible representation for the C_{3v} point group. It is given in the table below without derivation, but it is easy to demonstrate that it satisfies the group multiplication table.

C_{3v}			**E**	**C$_3$**
Γ_1	A_1	1	1	1
Γ_2	A_2	1	1	1
Γ_3	E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$

C_{3v}		σ_v	σ_v'	σ_v''
Γ_1	A_1	1	1	1
Γ_2	A_2	-1	-1	-1
Γ_3	E	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$

This page titled 3.6: Representations is shared under a CC BY-NC-SA 4.0 license and was authored, remixed, and/or curated by Patrick Fleming.