CHAPTER III

APPLICATION

Symmetry groups

Most simple molecules will have a certain degree of symmetry; that is, there will be certain transformations of coordinates which leave the atoms of the molecule in a configuration in space which is indistinguishable from the former configuration. The possible transformations of this type will be either rotation about an axis of symmetry, reflection in a plane of symmetry, inversion in a center of symmetry, or various combinations of these transformations. If two such transformations are carried out successively, the configuration will be that which could be obtained from some other transformation.

The set of transformations which do not alter the configuration thus forms a group, the group of the symmetry operations.

The notation used for the operators which transform a symmetrical configuration into itself is the following:

E = the identity operation, which leave each particle in its original position.

C_n = rotation about an axis of symmetry by an angle $\frac{2\pi}{n}$.

σ = reflection in a plane of symmetry. The symmetry planes are further classified as follows. If the plane is perpendicular to the principal axis of symmetry (the axis with the largest value of n), reflection in this plane is denoted by σ_h. If the plane contains the principal axis, reflection in this plane is denoted by σ_v. If there are axes with n = 2 perpendicular to the principal axis, and if the plane contains the principal axis and bisects the angle between two of these 2-fold axes, reflection in this plane is designated by σ_d.

S_n = rotation about an axis by $\frac{2\pi}{n}$ followed by a reflection in a plane perpendicular to the axis of rotation.

i = inversion in a center of symmetry.

The symmetry groups are designated by the following notation. We may divide them into three main types:

1. The rotation groups. These are symmetry groups which have one symmetry axis which is of a higher degree than any other symmetry axis. This axis is considered to be the z coordinate axis. The following groups belong to this general class:

(a) the molecule posseses an axis of symmetry only. The groups of interest are $C_1, C_2, C_3, C_4, C_5, C_6$.

(b) the molecule has the symmetry operations C_n and σ_v. The possible groups are $C_{2v}, C_{3v}, C_{4v}, C_{5v}, C_{6v}$.

(c) The molecule has the symmetry operation S_n.

The possible groups are S_2, S_4, S_6 .

(d) The molecule has the symmetry operations C_n and σ_h. The possible groups are $C_{1h}, C_{2h}, C_{3h}, C_{4h}, C_{5h}, C_{6h}$.

(e) The molecule has 2n 2-fold axes perpendicular to the principal n-fold axis. These axes are denoted by C_2', C_2'' etc. The notation for this type of group is D_n. The possible groups are D_2, D_3, D_4, D_5, D_6.

(f) The molecule has the symmetry operations D_n and σ_d. The possible groups of interest are D_{2d}, D_{3d}.

(g) The molecule has the symmetry operations D_n, σ_d, and σ_h. The possible groups are $D_{2h}, D_{3h}, D_{4h}, D_{5h}, D_{6h}$.

A number of the above groups can be expressed quite simply as the combination of some other group of symmetry operations plus the inversion i. These are

$$C_{4h} = C_4 \times i \qquad D_{2h} = D_2 \times i$$
$$C_{6h} = C_6 \times i \qquad D_{4h} = D_4 \times i$$
$$S_6 = C_3 \times i \qquad D_{6h} = D_6 \times i$$
$$D_{3d} = D_3 \times i$$

2. Groups of higher symmetry. These are groups which have no unique axis of high symmetry but which have more than one n-fold axis where $n > 2$. The groups of interest are:

T = the group of operations which sends a regular tetrahedron into itself. $T_h = T \times i$.

O = the group of operations which sends a cube or a regular octahedron into itself. $O_h = O \times i$.

T_d = the symmetry group of CH_4.

3. Groups with the symmetry operation C_∞.

$C_{\infty v}$ = the group of the symmetry operations of a heteronuclear diatomic molecule.

$D_{\infty h}$ = the group of the symmetry operations of a homonuclear diatomic molecule.

Normal vibration modes of the systems with 5 masses

The normal vibrations of water (H_2O) and acetylene (C_2H_2) with three and four atoms respectively, are so well known to us.

We shall now proceed to the discussion of several examples with 5 masses.

Example 1: Consider first the system with 5 masses, lying in the xy - plane. The center mass is M, and the other four masses equal to m. The dimensions of the system are shown as in Fig.3.

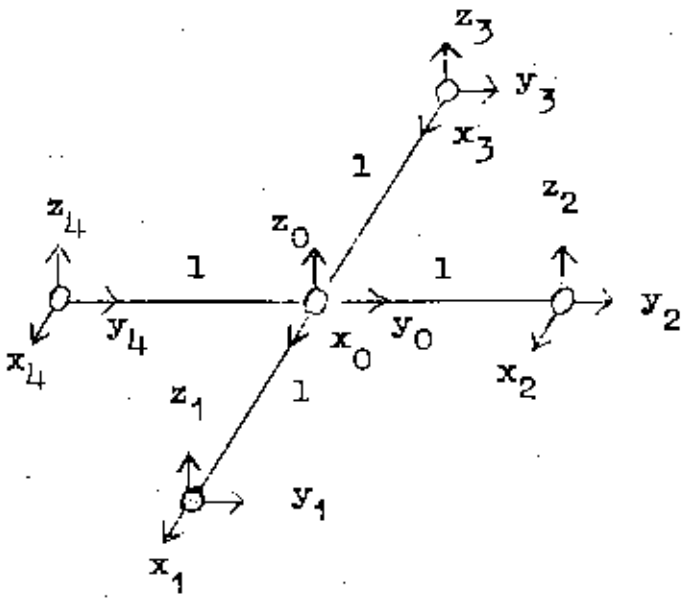

Figure 3. Original displacement coordinates of the system belonging to D_{4h}.

3N = 15 cartesian displacement coordinates x_0, y_0, z_0 ....., x_4, y_4, z_4 are needed to define the positions of 5 masses, where N is the number of masses.

By considering the symmetry operations applied to this system, we see that the system belongs to the group D_{4h} which can be expressed as $D_4 \times i$.

The application of a symmetry operation yields a new set of displacement coordinates x_0', y_0', z_0', ..., x_4', y_4', z_4' related to the old set by a number of linear equations. These symmetry operations are E, C_2, C_4, C_2', C_2'', and i,

where C_2 = rotation through 180° about the z - axis,

C_4 = rotation through 90° about the z - axis,

C_2' = rotation through 180° about one of the two diagonal lines in the xy - plane,

C_2'' = rotation through 180° about one of the coordinate axes x or y.

For C_2:

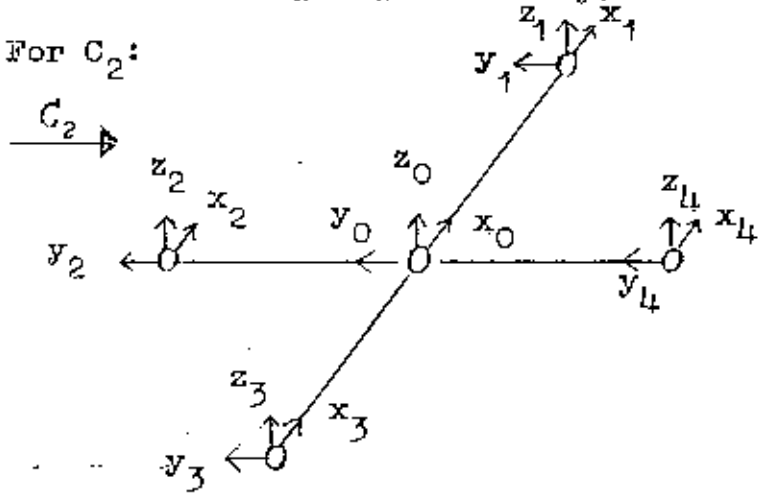

Figure 4. Displacement coordinates under the operation C_2.

We have the set of linear equations

$$
\begin{array}{llllll}
 & x_0' = -x_0 & x_1' = -x_3 & x_2' = -x_4 \\
C_2: & y_0' = -y_0 & y_1' = -y_3 & y_2' = -y_4 \\
 & z_0' = z_0 & z_1' = -z_3 & z_2' = z_4 \\
 & x_3' = -x_1 & x_4' = -x_2 & \\
 & y_3' = -y_1 & y_4' = -y_2 & \\
 & z_3' = z_1 & z_4' = z_2. &
\end{array}
$$

The matrix representation for C_2 is

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

For C_4:

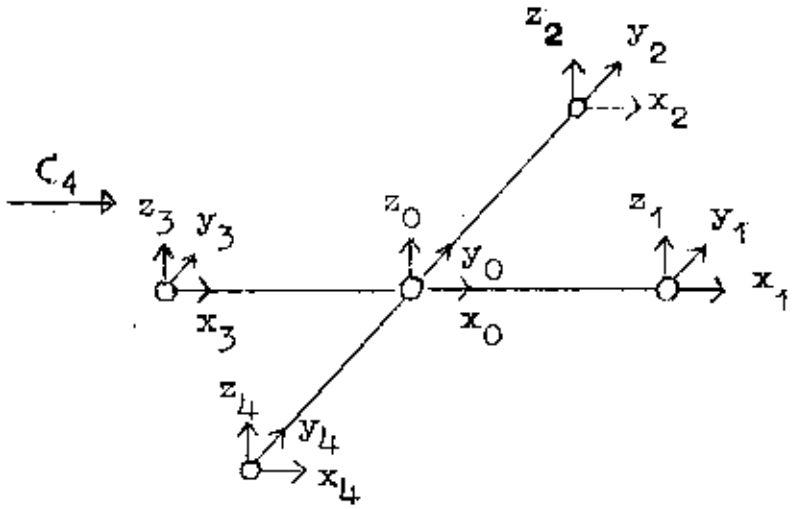

Figure 5. Displacement coordinates under the operation C_4.

The set of transformed coordinates is

$$
\begin{array}{llllll}
 & x_0' = y_0 & x_1' = y_2 & & x_2' = y_3 & \\
C_4: & y_0' = -x_0 & y_1' = -x_2 & & y_2' = -x_3 & \\
 & z_0' = z_0 & z_1' = z_2 & & z_2' = z_3 & \\
 & x_3' = y_4 & x_4' = y_1 & & & \\
 & y_3' = -x_4 & y_4' = -x_1 & & & \\
 & z_3' = z_4 & z_4' = z_1 . & & &
\end{array}
$$

The matrix representation for C_4 is

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

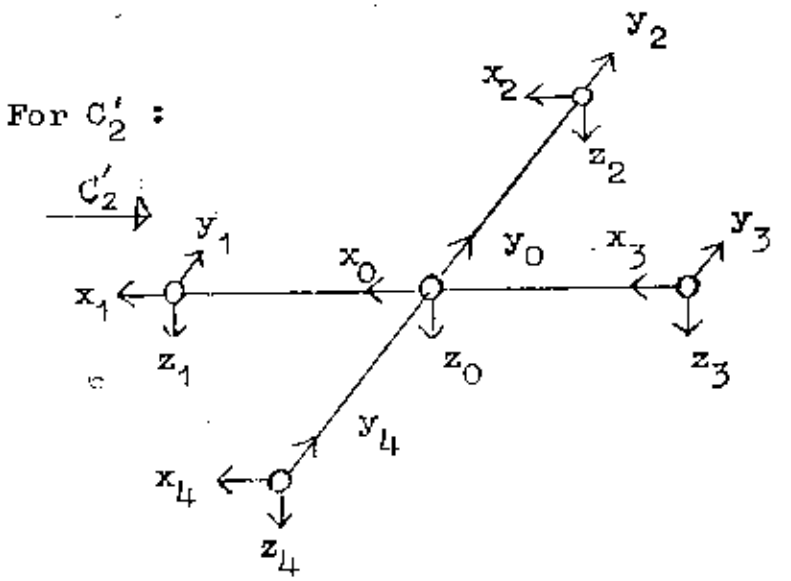

Figure 6. Displacement coordinates under the operation C_2' .

The set of transformed coordinates is

C_2' : $x_0' = -y_0$ $x_1' = -y_4$ $x_2' = -y_3$

$y_0' = -x_0$ $y_1' = -x_4$ $y_2' = -x_3$.

$z_0' = -z_0$ $z_1' = -z_4$ $z_2' = -z_3$

$x_3' = -y_2$ $x_4' = -y_1$

$y_3' = -x_2$ $y_4' = -x_1$

$z_3' = -z_2$ $z_4' = -z_1$.

The matrix representation for C_2' is

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

For C_2'' :

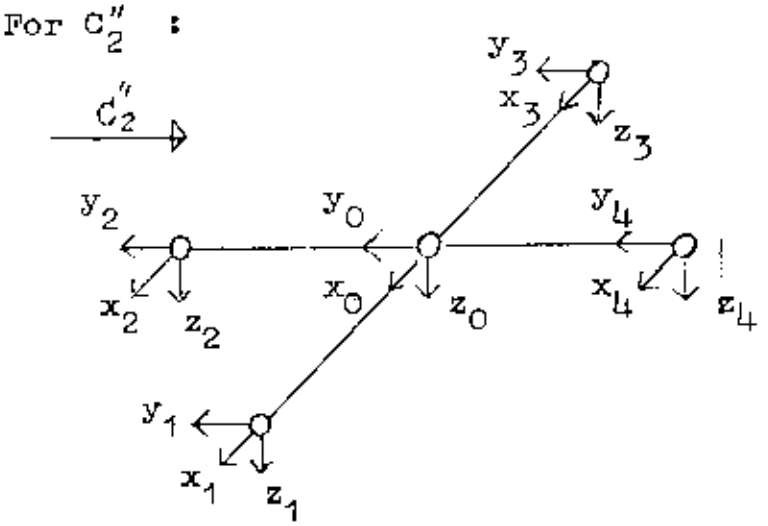

Figure 7. Displacement coordinates under the operation C_2'' .

The set of transformed coordinates is

$$C_2'' : \begin{array}{lll} x_0' = x_0 & x_1' = x_1 & x_2' = x_4 \\ y_0' = -y_0 & y_1' = -y_1 & y_2' = -y_4 \\ z_0' = -z_0 & z_1' = -z_1 & z_2' = -z_4 \\ x_3' = x_3 & x_4' = x_2 & \\ y_3' = -y_3 & y_4' = -y_2 & \\ z_3' = -z_3 & z_4' = -z_2. & \end{array}$$

The matrix representation for C_2'' is

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

Clearly, the matrix representation for E is a diagonal matrix, with diagonal elements all equal to + 1.

The sum of the diagonal elements of a square matrix is known as the character of the matrix. Therefore, the characters of the operations E, C_2, C_4 , C_2' , C_2'' are

$\chi(E) = 15$, $\chi(C_2) = -1$, $\chi(C_4) = 1$,

$\chi(C_2') = -1$, $\chi(C_2'') = -3$

Note that the character $\chi(E)$ of the identity operation necessarily equals the number of coordinates forming the basis of the representation.

After considering the matrix representations for E, C_2, C_4, C_2' , and C_2'' , we have the following 3× 3 matrix equations:

$$E\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} \qquad C_2\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x \\ \bar{y} \\ z \end{Bmatrix}$$

$$C_4\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} \qquad C_2'\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix}$$

$$C_2''\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix}.$$

The various rotations may be indicated by curved arrows as indicated in Fig. 8 . Operating on these arrows with the symmetry operations , we have

$$E\begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} \qquad C_2\begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix}$$

$$C_4\begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} \qquad C_2'\begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix}$$

$$C_2''\begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{Bmatrix} R_x \\ R_y \\ R_z \end{Bmatrix}.$$

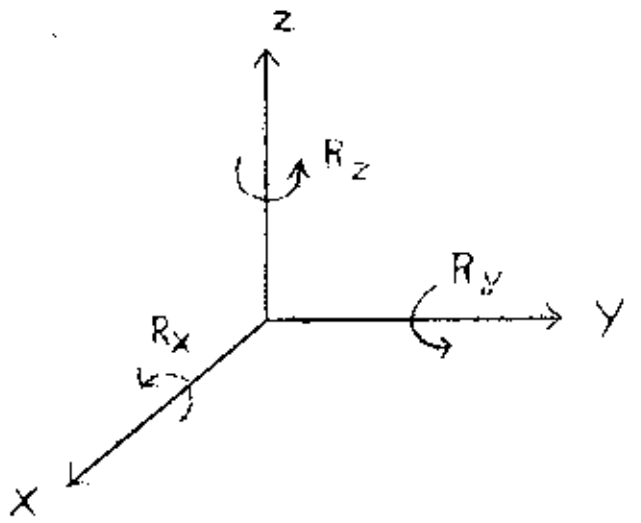

Figure 8. Diagram, showing the rotations, R_x, R_y, and R_z.

The character table for the group D_{4h} can be constructed as follows :

We first write the character table for D_4 and then apply the inversion i .

D_4			E	C_2	$2C_4$	$2C_2'$	$2C_2''$
x^2+y^2, z^2		A_1	1	1	1	1	1
	R_z, z	A_2	1	1	1	-1	-1
		B_1	1	1	-1	1	-1
		B_2	1	1	-1	-1	1
(xz , yz)	(x,y)	E	2	-2	0	0	0
(x^2-y^2, xy)	(R_x, R_y)						

Table 4. Character table for the group D_4.

The irreducible representations A and B always refer to one - dimensional representations, E refers to two - dimensional representations. Pairs of complex-conjugate representations are bracketed together and labeled as a two-dimensional representation E , because time-reversal symmetry makes them degenerate. The subscripts g and u, for gerade and ungerade, indicate even and odd representations under inversion. Inaddition to these representation labels, we also indicate the transformation properties of the coordinates x, y, z, of various bilinear combinations of coordinates, and of the infinitesimal rotations R_x, R_y, and R_z.

$D_{4h} = D_4 \times i$			E	C_2	$2C_4$	$2C_2'$	$2C_2''$	iE	iC_2	$2iC_4$	$2iC_2'$	$2iC_2''$
x^2+y^2, z^2		A_{1g}	1	1	1	1	1	1	1	1	1	1
		A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
	R_z	A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
	z	A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
		B_{1g}	1	1	−1	1	−1	1	1	−1	1	−1
		B_{1u}	1	1	−1	1	−1	−1	−1	1	−1	1
		B_{2g}	1	1	−1	−1	1	1	1	−1	−1	1
		B_{2u}	1	1	−1	−1	1	−1	−1	1	1	−1
(x^2-y^2, xy)	(R_x, R_y)	E_g	2	−2	0	0	0	2	−2	0	0	0
(xz, yz)	(x, y)	E_u	2	−2	0	0	0	−2	2	0	0	0
Γ_{3N}			15	−1	1	−1	−3	−3	5	−1	1	3

Table 5. Character table for the group D_{4h}.

Breaking the reducible representation down into its irreducible components, we have

$$\Gamma_{3N} = A_{1g} + A_{2g} + 2A_{2u} + B_{1g} + B_{1u} + B_{2g} + E_g + 3E_u \quad \ldots\ldots (3.1)$$

Certain of the normal coordinates which belong to these irreducible representations represent translational and rotational motion. We have for the representation which has these motions as its basis

$$\Gamma_{t,r} = A_{2g} + A_{2u} + E_g + E_u \quad \ldots\ldots (3.2)$$

subtracting $\Gamma_{t,r}$ from Γ_{3N}, we obtain

$$\Gamma_{vib} = A_{1g} + A_{2u} + B_{1g} + B_{1u} + B_{2g} + 2E_u \quad \ldots\ldots (3.3)$$

as the representation which has the vibrational motions as its basis.

Example 2: As in example 1., but the dimensions of the system are shown as in Fig. 9.

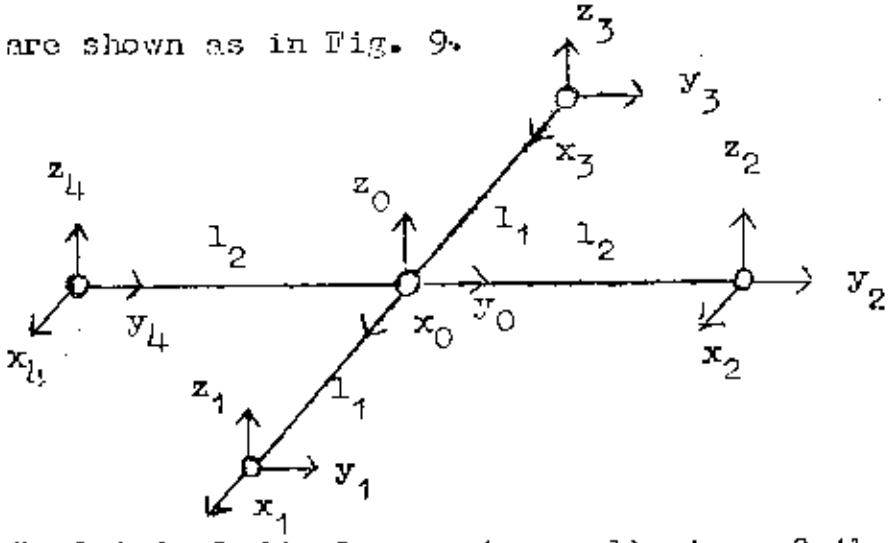

Figure 9. Original displacement coordinates of the system belonging to D_{2h}.

In the same manner as in example 1 , this system belongs to the group D_{2h} which can be expressed as $D_2 \times i$.

The symmetry operations applied to the system are:

E = identity operation,

C_2^z = rotation through 180° about the z - axis,

C_2^y = rotation through 180° about the y - axis,

C_2^x = rotation through 180° about the x - axis,

i = inversion in a center of symmetry.

The character table for the group D_{2h} is as follows:

$D_{2h} = D_2 \times i$			E	C_2^z	C_2^y	C_2^x	i	$\sigma_s(xy)$	$\sigma(zx)$	$\sigma(yz)$
x^2, y^2, z^2		A_{1g}	1	1	1	1	1	1	1	1
		A_{1u}	1	1	1	1	−1	−1	−1	−1
xy	R_z	B_{1g}	1	1	−1	−1	1	1	−1	−1
z		B_{1u}	1	1	−1	−1	−1	−1	1	1
xz	R_y	B_{2g}	1	−1	1	−1	1	−1	1	−1
y		B_{2u}	1	−1	1	−1	−1	1	−1	1
yz	R_x	B_{3g}	1	−1	−1	1	−1	−1	1	1
x		B_{3u}	1	−1	−1	1	−1	1	1	−1
		Γ_{3N}	15	−1	−3	−3	−3	5	3	3

Table 6. Character table for the group D_{2h}.

Breaking the reducible representation down into its irreducible components, we have

$$\Gamma_{3N} = 2A_{1g} + 2B_{1g} + 3B_{1u} + B_{2g} + 3B_{2u} + B_{3g} + 3B_{3u} \quad \ldots\ldots (3.4)$$

Finally, we obtain

$$\Gamma_{vib} = 2A_{1g} + B_{1g} + 2B_{1u} + 2B_{2u} + 2B_{3u} \quad \ldots\ldots\ldots\ldots (3.5)$$