CHAPTER II

GROUP THEORY

Definition of group

A set of elements A, B, C, etc., is called a group under the operation * if it satisfies the following conditions:

(1) If A and B are elements of the set, then so is $A * B$; i.e., the set is closed under the operation * .

(2) The associative law holds; that is, $A * (B * C) = (A * B) * C$.

(3) The set contains an element E called the identity such that $A * E = E * A = A$ for every element A of the set.

(4) If A is in the set, then so is an element B such that $A * B = B * A = E$. The element B is called the inverse of A, and is denoted by A^{-1}.

Two elements A, B of a group are said to commute with each other if $A * B = B * A$. If all elements of a group commute with one another the group is said to be commutative or abelian. The number of elements in a group is called the order of the group. A group which contains a finite number of elements is called the finite group.

Examples

(1) The set of all positive and negative integers including zero. In this case, ordinary addition serves as the group operation, zero serves as the identity, and $-n$ is the inverse of n. Clearly the set is closed, and the associative law is obeyed.

(2) Let us consider the symmetrical figure formed by three points at the corners of an equilateral triangle, as in Figure 2. The operations which send this figure into itself are:

1. The identity operation E, which leaves each point unchanged.

2. Operation A, which is a reflection in the yz-plane

3. B - reflection in the plane passing through the point b and perpendicular to the line joining a and c.

4. C - reflection in the plane passing through c and perpendicular to the line joining a and b.

5. D - clockwise rotation through 120° about the z-axis.

6. F - counterclockwise rotation through 120° about the z-axis.

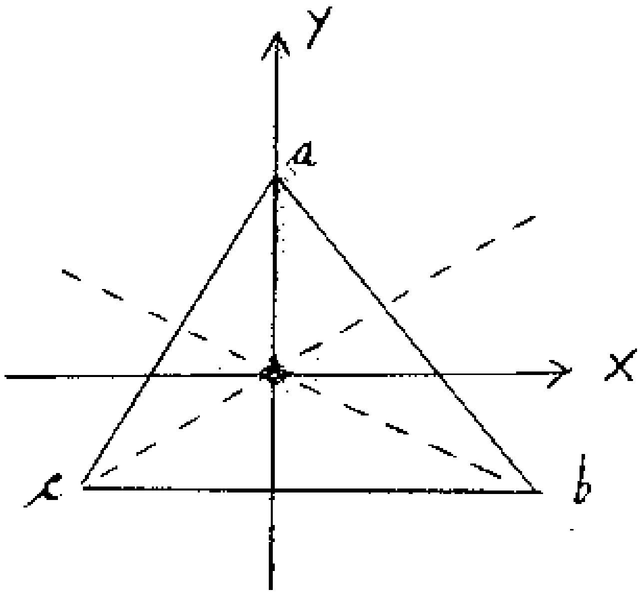

Figure 2. **Symmetry axes of equilateral triangle.**

Other symmetry operations are possible, but they are all equivalent to one of the operations given above. The successive application of any two of the operations listed above will be equivalent to same single operation.

If we work out all possible products of two operations, we obtain the following multiplication table, Table 1, where the operation which is to be applied to the figure first is written across the top of the table. The set of operations E, A, B, C, D and F forms a group, and Table 1. is known as the multiplication table for this group. Here the order of the group is 6.

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

Table 1. Multiplication table

Subgroups

Let G be a group. If we select from the elements of the group G a subset H and H is also a group, H is said to be a subgroup of the group G.

Isomorphism and homomorphism

def.

Two groups G_1, G_2 are called isomorphic if there exists a one-to-one correspondence between the elements A_1, B_1, ... of G_1 and those A_2, B_2, ... of G_2, such that $A_1 * B_1 = C_1$ implies $A_2 * B_2 = C_2$ and vice versa. Note that two groups having the same multiplication table are isomorphic.

Two groups G_1, G_2 are called homomorphic if there exists a correspondence between the elements of the two groups of the sort $A \longleftrightarrow A_1'$, A_2' , ... By this we mean that, if $A * B = C$, then the product of any A_i' with any B_j'

will be a member of the set C_k'. In general, a homomorphism is a many-to-one correspondence, as indicated here.

The general principles of group theory

The set of operations which send a symmetrical figure into itself are said to form a group.

Let us consider example (2) above, we have three distinct types of operations: the identity operation E; the reflections A, B, and C; and the rotations D and F. We say that each of these sets of elements forms a class; that is, E forms a class by itself, A,B, and C form a class, and D and F form a class. Usually the geometric considerations will enable us to pick out the classes; more precisely, two elements P and Q which satisfy the relation $X^{-1}PX = P$ or Q, where X is any element of the group and X^{-1} is its reciprocal, are said to belong to the same class. If the group is Abelian, then $X^{-1}PX = X^{-1}XP = P$ for all X's and P's. Each element of the group then forms a class by itself, and the number of the classes is equal to the number of elements. The concept of a class of operations has the following geometric meaning. If two operations belong to the same class, it is posible to pick out a new coordinate system in which one operation is replaced by the other.

Representation of groups

Any set of elements which multiply according to the group multiplication table is said to form a representation Γ of the group.

From example (2) given above, we see that the sets of number assigned to the various elements in the following way form representations of the group.

E	A	B	C	D	F
1	1	1	1	1	1
1	−1	−1	−1	1	1

The corresponding matrices will also form a representation of the group if we replace ordinary multiplication by matrix multiplication. If we denote by [E], [A], [B], [C], [D], [F], the matrices of the transformations of coordinates associated with the corresponding operations, we see that these matrices form a representation of the group. That is, the product of, say, A and B is AB = D; the product of the matrices [A] and [B] must therefore be [A] [B] = [D], so that the matrices multiply according to the group multiplication table. We have therefore found three matrix representations;

	E	A	B	C	D	F
Γ_1	1	1	1	1	1	1
Γ_2	1	−1	−1	−1	1	1
Γ_3	$\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$	$\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix}$	$\begin{bmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{bmatrix}$	$\begin{bmatrix}\frac{1}{2} & \frac{\sqrt{3}}{2}\\ \frac{\sqrt{3}}{2} & -\frac{1}{2}\end{bmatrix}$	$\begin{bmatrix}-\frac{1}{2} & \frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{bmatrix}$	$\begin{bmatrix}-\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ \frac{\sqrt{3}}{2} & -\frac{1}{2}\end{bmatrix}$

Table 2. Matrix representation.

In Γ_3, the matrices [E] and [A] can be written down immediately. [D] and [F] are obtained from $\begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}$ by inserting the proper value of θ; [B] and [C] can then be found by means of the group multiplication table and the rule for matrix multiplication.

<u>Group characters</u>

The characters of a group are the traces of the matrices in the representations of the group. We remember that the trace of a matrix is the sum of the diagonal elements of the matrix, and as it is unchanged by conjugation of the matrix it must be the same for all the matrices of the same class in a given representation. The use of the symbol χ for group characters is conventional. The character of any one - dimensional representation is, of course, the same as the representation itself.

<u>Reducible and irreducible representations</u>

The transformations of the type $[A'] = [B]^{-1} [A] [B]$ are called similarity transformation. The matrix representation which is reduced by the similarity transformation is said to be reducible. If it is not possible to find a similarity transformation which will further reduce all the matrices of a given representation, the representation is said to be irreducible.

The representations $\Gamma_1, \Gamma_2, \Gamma_3$ given above are allirreducible. Since matrices representing transformation of interest to us are unitary, we may restrict ourselves to representations which involve only unitary matrices and to similarity transformations with unitary matrices.

Two irreducible representations which differ only by a similarity transformation are said to be equivalent. Since the number of irreducible representations is equal to the number of classes, the characters can be set out in a square table. It is convenient to display the characters of the various representations in a character table for any given group. The columns are labeled by the various classes. The rows are labeled by the irreducible representations. Thus, from Table 2., we have the character table:

	E	A, B, C	D, F
Γ_1	1	1	1
Γ_2	1	-1	1
Γ_3	2	0	-1

Table 3. **Illustrative character table.**

We denote Γ_i (R) the matrix corresponding to the operation R of the ith irreducible representation, and by $\Gamma_i(R)_{mn}$ the mnth component of this matrix.

Theorems[1]

(G_1) The set of vectors $\sqrt{\frac{l_i}{h}}\ \Gamma_i(R)_{mn}$ forms an orthonormal set, that is

$$\sum_R \Gamma_i(R)_{mn} \sqrt{\frac{l_i}{h}}\ \Gamma_j(R)_{m'n'} \sqrt{\frac{l_j}{h}} = \delta_{ij}\ \delta_{mm'}\ \delta_{nn'}\ , \quad \ldots\ldots(2.1)$$

where l_i and l_j are the dimensions of the representations and h is the order of the group.

Before we begin the actual proof of the orthogonality relations, we need several preliminary theorems.

Theorem 1. If we have two sets of variables $x_1' \ldots x_n'$ and $y_1' \ldots y_m'$, then every bilinear form

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[1]**Eyring, Henry., Walter, John., and Kimball, George E. Quantum Chemistry. (New York: John Wiley and Sons, Inc., 1944), pp.** 371–376.

$$f = \sum_{i=1}^{n} \sum_{j=1}^{m} c_{ij}\, x_i'\, y_j' \qquad \ldots\ldots\ldots\ldots(2.2)$$

of these variables can be reduced to the normal form

$$f = \sum_{k=1}^{r} x_k y_k \qquad \ldots\ldots\ldots\ldots(2.3)$$

where $r \leq n$, $r \leq m$, by a suitable linear transformation of the variables x_i' and y_j'.

<u>Proof</u> The product

$$\frac{1}{c_{11}} \left(\sum_{i=1}^{n} c_{i1}\, x_i' \right) \left(\sum_{j=1}^{m} c_{1j}\, y_j' \right) \qquad \ldots\ldots\ldots\ldots(2.4)$$

contain all the terms in f which involve either x_1' or y_1'.

If we make the substitutions

$$x_1 = \frac{1}{c_{11}} \sum_{i=1}^{n} c_{i1}\, x_i' \qquad \ldots\ldots\ldots\ldots(2.5)$$

$$y_1 = \frac{1}{c_{11}} \sum_{j=1}^{m} \alpha_{1j}\, y_j'$$

We may write f as

$$f = x_1 y_1 + \sum_{i=2}^{n} \sum_{j=2}^{m} d_{ij}\, x_i'\, y_j' \qquad \ldots\ldots\ldots\ldots(2.6)$$

We can, without loss of generality, assume that $n < m$. After (n-1) substitution of the type (2.5), we will have obtained the result

$$f = x_1 y_1 + x_2 y_2 + \ldots + x_{n-1}\, y_{n-1} + \sum_{j=n}^{m} g_{nj}\, x_n'\, y_j' \quad \ldots(2.7)$$

We now make the final substitutions

$$x_n = x_n', \; y_n = \sum_{j=n}^{m} g_{nj} \, y_j' \; , \; y_j = y_j' \; (j > n)$$

Equation (2.7) then reduces to

$$f = \sum_{i=1} x_i \, y_i \qquad \text{...........(2.8)}$$

which is the desired result.

Let us now take a set of variables $x'_1 \ldots\ldots x'_n$ which form a basis for an irreducible representation $\Gamma_{x'}$ of a group. We also take a set of variables $y'_1 \ldots\ldots y'_m$ which form a basis for an irreducible representation $\Gamma_{y'}$ of the same group. We have then

<u>Theorem 2</u>. If $\Gamma_{x'}$ and $\Gamma_{y'}$ are two irreducible representations of a group there is no bilinear form of the variables x_i' and y_j' which is always invariant when both the x_i' and the y_j' are subjected to some operation R of the group unless $\Gamma_{x'}$ is identical with $\Gamma_{y'}$.

<u>Proof</u> We shall prove this theorem only for the type of groups in which we have been interested, namely, those representing transformations of coordinates. The corresponding matrix representations involve only unitary matrices. According to Theorem 1, any bilinear form

$$f = \sum_{i=1}^{n} \sum_{j=1}^{m} C_{ij} \, x_i' \, y_j' \qquad \text{...........(2.9)}$$

can be reduced to the form

$$f = \sum_{k=1}^{r} x_k y_k \qquad \text{..........(2.10)}$$

by a suitable transformation. We consider that the matrices of the representations $\Gamma_{x'}$ and $\Gamma_{y'}$ have been subjected to the same transformation, so that we have obtained the corresponding new representations Γ_x and Γ_y which have the x's and y's as their bases. We now require that f be invariant when both the x's and the y's have been operated on by some operation R of the group.

$$Rx_k = \sum_{s=1}^{n} \Gamma_x(R)_{sk}\, x_s \qquad \text{..........(2.11)}$$

$$Ry_k = \sum_{t=1}^{m} \Gamma_y(R)_{tk}\, y_t$$

If we operate on the x's only in equation (2.10), we have

$$f = y_1 \sum_{s=1}^{n} \Gamma_x(R)_{s1}\, x_s + y_2 \sum_{s=1}^{n} \Gamma_x(R)_{s2}\, x_s + \ldots + y_r \sum_{s=1}^{n} \Gamma_x(R)_{sr}\, x_s \qquad \text{..........(2.12)}$$

Arranging this according to the x's we have

$$f = x_1 \sum_{k=1}^{r} \Gamma_x(R)_{1k}\, y_k + \ldots\ldots + x_n \sum_{k=1}^{r} \Gamma_x(R)_{nk}\, y_k \qquad \text{.....(2.13)}$$

When we operate on the y's, equation (2.13) must reduce to equation (2.10). This requires that

$$\sum_{k=1}^{r} \Gamma_x(R)_{ik}\, R\, y_k = y_i, \quad i = 1 \ldots\ldots r$$

which is equivalent to the requirement that

$$R \sum_{k=1}^{r} \Gamma_x (R)_{ik}\, y_k \;=\; y_i$$

or
$$R^{-1} y_i \;=\; \sum_{k=1}^{r} \Gamma_x (R)_{ik}\, y_k, \quad i = 1 \ldots\ldots r \qquad \ldots\ldots(2.14)$$

For the real unitary matrix representations we have been considering, the matrix of the inverse transformation is obtained from the original matrix by simply interchanging rows and columns. By definition, therefore

$$R^{-1} y_i \;=\; \sum_{k=1}^{m} \Gamma_y (R)_{ik}\, y_k\,, \quad i = 1 \ldots\ldots m \qquad \ldots\ldots(2.15)$$

Comparing (2.14) and (2.15), we see that (2.10) will be invariant only if $m = r$. By interchanging the order of operations, we could prove in the same way that (2.10) will be invariant only if $n = r$.

Again comparing (2.15) and (2.14), we see that (2.10) is invariant only if

$$\Gamma_x(R)_{ik} = \Gamma_y(R)_{ik} \quad \text{for } i,\ k = 1 \ldots\ldots r.$$

Therefore equation (2.10) is invariant only if Γ_x and Γ_y are identical.

<u>Theorem 3</u>. If Γ_x is not identical with Γ_y, then

$$\sum_R \Gamma_x (R)_{ij}\, \Gamma_y (R)_{kl} \;=\; 0$$

for all values of i, j, k, l.

<u>Proof</u> From the definition of the direct product, we see that the mn functions $x_s y_t$ form a basis for a representation $\Gamma_x \Gamma_y$ of the group of dimension mn.

If we denote these mn functions by $z_1, \ldots. z_r$ $(r = mn)$ and the corresponding representation by

$$\Gamma_z = \Gamma_x \Gamma_y,$$

then
$$\Gamma_z(R) = \Gamma_x(R)_{ij} \Gamma_y(R)_{kl}$$

$$(i, j = 1 \ldots . n, \ k, \ l = 1 \ldots \ldots m).$$

If we now operate on z_s by one of the operations R of the group, we have

$$R z_s = \sum_{t=1}^{r} \Gamma_z(R)_{ts} z_t \quad \ldots\ldots\ldots\ldots (2.16)$$

Summing over all the operations R of the group,

$$f = \sum_R R z_s = \sum_R \sum_{t=1}^{r} \Gamma_z(R)_{ts} z_t \quad \ldots\ldots\ldots\ldots (2.17)$$

Let Λ be any operation of the group. Then

$$\Lambda f = \sum_R \Lambda R z_s = \sum_R R z_s = f,$$

since ΛR is always an operation of the group and the operation by Λ merely changes the order of summation. Now f is a linear form of the z's, and hence a bilinear form of the x's and y's. But we have just seen that there is no such form f which is invariant under an operation of the group.

Since $Af = f$, we must conclude that f is identically zero. This can be true only if $\sum_R \Gamma_z(R)_{ts}$ is identically zero for all values of t and s.

Proof of (G_1)

The function $f = \sum_{k=1}^{l} x_k y_k$ is invariant. We operate on f with some operation R, sum over all operations of the group, obtaining

$$\sum_R Rf = \sum_R \sum_{k=1}^{l} \sum_{s=1}^{l} \sum_{t=1}^{l} \Gamma(R)_{sk}\, \Gamma(R)_{tk}\, x_s y_t = hf \quad \ldots\ldots(2.18)$$

The coefficient of $x_s y_t$ must vanish if $s \neq t$, so we have the relation

$$\sum_R \Gamma(R)_{sk}\, \Gamma(R)_{tk} = 0 \,, \quad s \neq t \quad \ldots\ldots\ldots\ldots(2.19)$$

Now $\sum_R R^{-1} f = \sum_R R f$, since each operation is contained once and only once in both summations.

$$\sum_R Rf = \sum_R R^{-1} f = \sum_R \sum_{k=1}^{l} \sum_{s=1}^{l} \sum_{t=1}^{l} \Gamma(R)_{ks}\, \Gamma(R)_{kt}\, x_s\, y_t$$

which gives us the relation

$$\sum_R \Gamma(R)_{ks}\, \Gamma(R)_{kt} = 0, \quad s \neq t \quad \ldots\ldots\ldots\ldots(2.20)$$

Equation (2.18) is thus reduced to

$$\sum Rf = \sum_R \sum_{k=1}^{l} \sum_{j=1}^{l} \Gamma(R)_{jk}\, \Gamma(R)_{jk}\, x_j y_j = hf \quad \ldots\ldots(2.21)$$

This requires that

$$\sum_{R} \sum_{k=1} \Gamma(R)_{jk}\, \Gamma(R)_{jk} = h, \quad (j = 1....l) \quad ......(2.22)$$

Considering the inverse transformation, we also obtain

$$\sum_{R} \sum_{k=1} \Gamma(R)_{kj}\, \Gamma(R)_{kj} = h; \quad (j = 1,....l) \quad ....(2.23)$$

From (2.22) and (2.23), we see that $\sum_{R} \Gamma(R)_{jk}\, \Gamma(R)_{jk}$ is independent of both k and j.

Since $\sum_{k=1}^{l} (h_k) = h$ or $l h_k = h$, then

$$\sum_{R} \Gamma(R)_{jk}\, \Gamma(R)_{jk} = \frac{h}{l}$$

From Theorem 3.,

$$\sum_{R} \Gamma_x(R)_{ij}\, \Gamma_y(R)_{kl} = 0$$

Therefore we have

$$\sum_{R} \Gamma_i(R)_{mn} \sqrt{\frac{l_i}{h}}\; \Gamma_j(R)_{m'n'} \sqrt{\frac{l_j}{h}} = \delta_{ij}\, \delta_{mm'}\, \delta_{nn'}$$

<u>(G_2)</u> If there are c irreducible representations, each of dimension l_i, then $\sum_{i=1}^{c} l_i^2 = h$.

<u>Proof</u> From (G_1), we have

$$\sum_{R} \Gamma_i(R)_{mn} \sqrt{\frac{l_i}{h}}\; \Gamma_j(R)_{m'n'} \sqrt{\frac{l_j}{h}} = \delta_{ij}\, \delta_{mm'}\, \delta_{nn'}$$

Hence $\sum_{i=1}^{c} l_i^2 = h$

(G_3) The set of vectors $\chi_i(R_\rho)\sqrt{\frac{g_\rho}{h}}$ forms an orthonormal set, where g_ρ is the number of elements in class ρ, R_ρ is any one of the operations in this class, $\chi(R_\rho)$ is the corresponding character.

Proof From (G_1), we have

$$\sum_R \Gamma_i(R)_{mn} \sqrt{\frac{l_i}{h}}\, \Gamma_j(R)_{m'n'} \sqrt{\frac{l_j}{h}} = \delta_{ij}\ \delta_{mm'}\ \delta_{nn'}$$

Summing over m from 1 to l_i and over m' from 1 to l_j gives

$$\sum_R \chi_i(R)\ \chi_j(R) = \frac{h}{l_j}\ \delta_{ij} \sum_{m=1}^{l_i} \sum_{m'=1}^{l_j} \delta_{mm'}$$

$$= \frac{h}{l_j}\ \delta_{ij} \sum_{m'=1}^{l_j} 1$$

$$= h\ \delta_{ij} \qquad \text{...........(2.24)}$$

Since the characters of all matrices of a given representation which correspond to operations in the same class are equal. Equation (2.24) can be written as

$$\sum_{\rho=1}^{k} \chi_i(R_\rho)\chi_j(R_\rho)\ g_\rho = h\delta_{ij},$$ where k is the number of classes

or $$\sum_{\rho=1} \chi_i(R_\rho) \sqrt{\frac{g_\rho}{h}}\ \chi_j\ (R_\rho) \sqrt{\frac{g_\rho}{h}} = \delta_{ij} \qquad \text{...........(2.25)}$$

(G_4) The number of non-equivalent irreducible representations is equal to the number of classes.

Proof The normalized characters $\chi_i(R_\rho)\sqrt{\frac{g_\rho}{h}}$ are therefore the components of a set of orthonormal vectors in k-dimensional space. Since there can be k such vectors, we see that the number of irreducible representations is equal to the number of classes.

Decomposition of reducible representations

Any reducible representation can be reduced to its irreducible representations by a suitable similarity transformation which leaves the character unchanged. Thus we can write for the character of a matrix R of the reducible representation the expression

$$\chi(R) = \sum_{j=1}^{k} a_j \chi_j(R) \qquad \ldots\ldots\ldots\ldots(2.26)$$

where a_j is the number of times the jth irreducible representation occurs in the reducible representation.

From (2.24) we have

$$\sum_R \chi(R)\chi_i(R) = \sum_R \sum_j a_j\chi_j(R)\ \chi_i\ (R) = ha_i \quad \ldots\ldots.(2.27)$$

so that the number of times the irreducible representation Γ_i occurs in the reducible representation is

$$a_i = \frac{1}{h} \sum_R \chi(R)\ \chi_i(R)$$

or
$$a_i = \frac{1}{h} \sum_{\rho=1}^{k} g_\rho\, \chi\ (R_\rho)\ \chi_i\ (R_\rho) \qquad \ldots\ldots\ldots\ldots(2.28)$$