Special Topics Course
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Representations of Groups

Recall that your Inorganic Chemistry class includes finding the irreducible representations and the character table of a point group corresponding to a molecule. This note covers a bit more details of this procedure.

Defining main notions. A **representation** of a group G is a mapping that maps elements of G to (finite or infinite) invertible matrices over a field. For applications in chemistry, a "field" is usually either set of real or complex numbers. So, for us, a representation is a mapping that maps group elements to real or complex matrices. If representation is denoted by ρ and g is an element of G, then $\rho(g)$ denotes a matrix corresponding to element g.

Recall that a matrix just a table with numbers in it. If you took a Linear Algebra course, you know how to multiply two matrices. If you did not take Linear Algebra but you took Calculus 3, recall the dot product of two vectors: the entry in (i, j)-th spot of the matrix AB is the dot product of i-th row of A with j-th column of B.

Note that the number of columns of A must be the same as number of rows in B if you want the product AB to be defined. We will be interested just in **square** matrices i.e. matrices with same number of rows and columns.

We are mapping group elements to **invertible** matrices. A matrix B is the inverse matrix of a matrix A if $AB = BA = I$ where I is the identity matrix. This matrix consists of 1's on main diagonal and zeros everywhere else. This explains the reason we are interested just in square matrices: if both products AB and BA are defined and equal to the same matrix I, both A and B have to be square.

If A has an inverse, then it is called **invertible.** The inverse is denoted by A^{-1}. The set of all invertible matrices is a group: it is closed, associative, identity is I, the inverse of A is A^{-1}.

More background. Representation theory is the branch of mathematics that studies properties of abstract groups via their representations as linear transformations of vector spaces (for us real or complex invertible matrices). Representation theory is important because it enables many group-theoretic problems to be reduced to problems in linear algebra (for us playing with matrices with numerical entries), which is a very well-understood theory. The term representation of a group is also used in a more general sense to mean any "description" of a group as a group of transformations of some mathematical object. More formally, a "description" means a mapping (homomorphism) from the group to the automorphism group of the object (for us from group to a set of matrices).

Example 1. Consider the cyclic group with 3 elements $C_3 = \langle a | a^3 = 1 \rangle = \{1, a, a^2\}$. Let u denote the complex number $e^{2\pi i/3}$. So $1, u, u^2 = e^{4\pi i/3}$ are 3 solutions of the equation $z^3 = 1$ in complex plane. One possible representation of C_3 is the following map.

$$1 \mapsto \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad a \mapsto \begin{bmatrix} 1 & 0 \\ 0 & u \end{bmatrix} \quad a^2 \mapsto \begin{bmatrix} 1 & 0 \\ 0 & u^2 \end{bmatrix}$$

Two representations ρ_1 and ρ_2 are said to be equivalent if the matrices only differ by a change of basis, i.e. if there exists a matrix A such that for all x in G: $\rho_1(x) = A\rho_2(x)A^{-1}$. For example, another representation of C_3 is given by:

$$1 \mapsto \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad a \mapsto \begin{bmatrix} u & 0 \\ 0 & 1 \end{bmatrix} \quad a^2 \mapsto \begin{bmatrix} u^2 & 0 \\ 0 & 1 \end{bmatrix}$$

This representation is equivalent to the one above.

The **character** of a representation ρ is the function χ that maps G to complex numbers by mapping the element g in G to the **trace** (the sum of the diagonal elements) of the matrix $\rho(g)$. For example, the character of the any of the two representations of C_3 given above is given by:

$$\chi(1) = 2, \quad \chi(a) = 1 + u, \quad \chi(a^2) = 1 + u^2.$$

We will be mostly interested in **irreducible representations**. A representation is irreducible if it is not a direct sum of its subrepresentations (think of it as representations that are not decomposable into smaller ones).

Another relevant concept is that of a conjugacy class of group elements. Two elements g, h are in the same **conjugacy class** if there exist an element x in the group such that $g = xhx^{-1}$. These classes partition all the elements of a group.

If g and h are members of G in the same conjugacy class, then $\chi(g) = \chi(h)$ for any character χ. The values of a character therefore have to be specified only for the different conjugacy classes of G.

The conjugacy classes are relevant because of the following rule.

(1) The number of irreducible representations of a group is equal to the number of conjugacy classes.

The characters of all the irreducible representations of a finite group form a character table - these are the tables that you use in Inorganic Chemistry class. **The conjugacy classes of elements are the heading row, irreducible representations are the heading column and the characters fill the main part of the table**. The sums of irreducible representations gives you all (reducible) representations of a group. This is the reason we are interested only in irreducible representations: we can obtain all the others just by knowing the irreducible ones.

The character table is always square, and the rows and columns are orthogonal with respect to certain dot products which allow one to compute character tables more easily.

The following rules are helpful when filling the character table.

(2) The first row of the character table always consists of 1s, and corresponds to the **trivial representation**. Trivial representation is the one mapping all the elements of G to 1 (i.e. a matrix with one row and one column with a single entry 1).

(3) If n is the order of the group, m the number of conjugacy classes and χ_i, $i = 1, \ldots, m$ all the characters of all the irreducible representations, then

$$\sum_{i=1}^{m} (\chi_i(1))^2 = n.$$

The value $\chi_i(1)$ corresponds to the *dimension* of the representation: the size of the matrices onto which the group elements are mapped. For example, the representation from the example above is 2-dimensional. So, the above formula can also be written as

$$\sum_{i=1}^{m}(\dim(\chi_i))^2 = n.$$

(4) If $g_1, \ldots, g_n$ are all group elements, then

$$\sum_{k=1}^{n}(\chi_i(g_k))^2 = n$$

and

$$\sum_{k=1}^{n} \chi_i(g_k)\chi_j(g_k) = 0 \text{ for any } i \neq j.$$

If m_j, $j = 1, \ldots, m$ are the numbers of elements in all the conjugacy classes with representative $g_j, j = 1, \ldots, m$, then the formula $\sum_{k=1}^{n}(\chi_i(g_k))^2 = n$ can also be written as

$$\sum_{j=1}^{m} m_j(\chi_i(g_j))^2 = n.$$

(5) If a group is abelian, the number of conjugacy classes is equal to the number of group elements. Indeed, for every g and x in G,

$$xgx^{-1} = xx^{-1}g = g$$

so every element is conjugated just to itself.

(6) G is abelian if and only if $\chi(1) = 1$ for every character χ. Thus, if the group G is abelian, all the irreducible representations are one dimensional (i.e. group elements will be represented by 1×1 matrices). Note that for one dimensional representations the character of a representation is the same as the representation itself.

(7) If a one dimensional representation with character χ maps a group element g of order n (i.e. $g^n = 1$) to a complex number z, then $z^n = 1$. So, z has to be one of n solution of the equation $z^n = 1$. Recall that the formula for the n-th roots of 1 is the following:

$$z_k = e^{\frac{2k\pi}{n}i} \quad \text{for} \quad k = 0, 1, \ldots, n-1.$$

As most of the point groups are cyclic, dihedral, product of two cyclic or product of cyclic and dihedral, we will be mostly interested in representations of those.

Character tables of cyclic groups. To determine the irreducible representation of C_n it is sufficient to know the character of the generator a. Since $a^n = 1$, the character $\chi(a)$ will be one of the n-th roots of 1.

For example, to obtain an irreducible representation of $C_3 = \langle a | a^3 = 1 \rangle$, it is sufficient to know the image of the generator a. Since this image has to be the third root of 1, there are three choices for the image of a. The image of a^2 is completely determined by those choices since it has to be the square of the image of a.

Recall that the equation $x^3 = 1$ has three solutions in the complex plane: 1, $u = e^{2\pi i/3} = \frac{-1}{2} + \frac{\sqrt{3}}{2}i$ and $u^2 = e^{4\pi/3} = \frac{-1}{2} - \frac{\sqrt{3}}{2}i$.

The trivial irreducible representation maps a to 1 and thus a^2 is mapped to 1 too. Two nontrivial irreducible representations of C_3 are

$$1 \mapsto 1, a \mapsto u, a^2 \mapsto u^2 \text{ and} 1 \mapsto 1, a \mapsto u^2, a^2 \mapsto u.$$

Denote their characters by χ_1 and χ_2. Thus the character table for C_3 is

	1	a	a^2
1	1	1	1
χ_1	1	u	u^2
χ_2	1	u^2	u

Note that the representation from Example 1 above is the direct sum of 1 and representation with character χ_1.

Let us look at the cyclic group C_4 now. Note that the solutions of $x^4 = 1$ are $1, i, -1, -i$. So, there are four choices for the image of a : 1, $i, -1$ and $-i$. The images of the other elements are completely determined by the image of a since the image of a^2 has to be the square of a and the image of a^3 is the cube of the image of a. The character table is given below.

C_4	1	a	a^2	a^3
1	1	1	1	1
χ_1	1	i	-1	$-i$
χ_2	1	-1	1	-1
χ_3	1	$-i$	-1	i

For C_5, let $u = e^{2\pi i/5}$. Then

C_5	1	a	a^2	a^3	a^4
1	1	1	1	1	1
χ_1	1	u	u^2	u^3	u^4
χ_2	1	u^2	u^4	u	u^3
χ_3	1	u^3	u	u^4	u^2
χ_4	1	u^4	u^3	u^2	u

Character tables of dihedral groups. Recall that $D_n = \langle a, b | a^n = 1, \quad b^2 = 1, \quad ba = a^{n-1}b\rangle$. This is the group of symmetries of regular polygon with n sides. The element a is rotation for $\frac{360}{n}$ degrees and all the elements $b, ab, a^2b, \ldots a^{n-1}b$ are various reflections. The pairs of elements $\{a, a^{n-1}\}, \{a^2, a^{n-2}\}$ etc are different conjugacy classes. If n is odd, the last is the class $\{a^{(n-1)/2}, a^{(n+1)/2}\}$ and all the reflections are in the same conjugacy class. So, there are $1 + \frac{n-1}{2} + 1 = \frac{n+3}{2}$ elements in the leading row.

If n is even, the pairs of elements $\{a, a^{n-1}\}, \{a^2, a^{n-2}\}, \ldots \{a^{(n-2)/2}, a^{(n+2)/2}\}, \{a^{n/2}\}$ are in different conjugacy classes. The reflections are conjugate either with b or with ab. So, there are $1+\frac{n}{2}+2 = \frac{n+6}{2}$ elements in the leading row.

Odd Case. Let us look at the case when n is odd first. D_n has two one dimensional representations that map a^i to 1 for all $i = 0, \ldots, n-1$ and b either to 1 or to -1. Two formulas of item (4) above rule out the other possible n-th roots of 1 as the images of a^i.

Then there are $\frac{n-1}{2}$ two dimensional irreducible representations that map a to the matrix $\begin{bmatrix} e^{2k\pi i/n} & 0 \\ 0 & e^{-2k\pi i/n} \end{bmatrix}$ for $k = 1, \ldots \frac{n-1}{2}$ and b to $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Thus the traces of these matrices are $e^{2k\pi i/n} + e^{-2k\pi i/n} = 2\cos\frac{2k\pi}{n}$ and 0 respectively. The images of other elements are determined by the images of the generators. For example, the image of ab will be the trace of the product of the matrices that are images of a and b.

Note that the formula (3) agrees with these numbers since $2(1)^2 + \frac{n-1}{2}(2)^2 = 2 + 2(n-1) = 2n$ which is the number of elements in D_n.

The character tables for D_3 and D_5 are given below.

D_3	1	a	b
1	1	1	1
χ_1	1	1	-1
χ_2	2	$2\cos\frac{2\pi}{3} = -1$	0

D_5	1	a	a^2	b
1	1	1	1	1
χ_1	1	1	1	-1
χ_2	2	$2\cos\frac{2\pi}{5}$	$2\cos\frac{4\pi}{5}$	0
χ_3	2	$2\cos\frac{4\pi}{5}$	$2\cos\frac{2\pi}{5}$	0

Even Case. Let n be even now. D_n has four one dimensional irreducible representations that map a to ± 1 and b to ± 1 in all four possible combinations. Two formulas of item (4) above rule out the other possible n-th roots of 1 as the images of a^i.

Then, there are $\frac{n}{2} - 1$ representations that map a to $\begin{bmatrix} e^{2k\pi i/n} & 0 \\ 0 & e^{-2k\pi i/n} \end{bmatrix}$ for $k = 1, \ldots \frac{n-2}{2}$ and b to $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ similarly to the case when n is odd. For example, the tables for D_2, D_4 and D_6 are given below.

D_2	1	a	b	ab
1	1	1	1	1
χ_1	1	-1	1	-1
χ_2	1	1	-1	-1
χ_3	1	-1	-1	1

D_4	1	a	a^2	b	ab
1	1	1	1	1	1
χ_1	1	-1	1	1	-1
χ_2	1	-1	1	-1	1
χ_3	1	1	1	-1	-1
χ_4	2	$2\cos(2\pi/4) = 0$	$2\cos(4\pi/4) = -2$	0	0

D_6	1	a	a^2	a^3	b	ab
1	1	1	1	1	1	1
χ_1	1	-1	1	-1	1	-1
χ_2	1	-1	1	-1	-1	1
χ_3	1	1	1	1	-1	-1
χ_4	2	$2\cos(2\pi/6) = 1$	$2\cos(4\pi/6) = -1$	$2\cos(6\pi/6) = -2$	0	0
χ_5	2	$2\cos(4\pi/6) = -1$	$2\cos(8\pi/6) = -1$	$2\cos(12\pi/6) = 2$	0	0

Representations of product of two groups. If G_1 and G_2 are represented by ρ_1 and ρ_2 with characters χ_1 and χ_2, then the direct product $G_1 \times G_2$ is represented by representation ρ given by the tensor product of matrices and the character of the product $G_1 \times G_2$ is $\chi_1 \cdot \chi_2$. This product is irreducible if (and only if) both χ_1 and χ_2 are irreducible.

For example, one nontrivial irreducible representation of C_2, determines 3 nontrivial irreducible representations of $C_2 \times C_2 = \{1, a, b, ab\}$.

C_2	1	a
1	1	1
χ	1	-1

C_2	1	b
1	1	1
χ	1	-1

$\longrightarrow$

$C_2 \times C_2$	1	a	b	ab
1	1	1	1	1
χ_1	1	-1	1	-1
χ_2	1	1	-1	-1
χ_3	1	-1	-1	1