3.8: Character and Character Tables

Most summaries of group theory do not give the full matrix specifications for each irreducible representation in each important point group. Rather, a very useful quantity is defined, called the **character**. An important property that elements of the same class will share is that they have the same character. As such, it is only necessary to show the character once for each class of operations in the group.

The character of an element is given by the sum of the diagonal elements of the matrix used to represent the symmetry operation.

$$\chi_i(R) = \sum_m \Gamma_i(R)_{mm}$$

C_{3v}	E	C_3	s_v
A_1	1	1	1
A_2	1	1	-1
E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \cos(2\pi/3) & -\sin(2\pi/3) \\ \sin(2\pi/3) & \cos(2\pi/3) \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

To evaluate the characters of each of the classes within each irreproducible representation, we need only generate a representation for one operation within each class. The three irreducible representations for some characteristic operators in each class can be expressed as follows:

Using the expressions above, the character table for the C_{3v} group can be expressed as

C_{3v}	E	$2\ C_3$	$3\ \sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Note that the character of the identity element is always given as the dimension of the matrices used in the irreducible representation.

$$\chi_i(E) = l_i$$

The GOT can be expressed in terms of characters.

$$\sum_R \chi_i(R)\chi_j(R) = h\delta_{ij}$$

This statement has a number of important and useful properties and consequences. One relationship deals with the sum of the squares of the characters of the identity elements.

$$\sum_i [\chi_i(E)]^2 = h$$

These expressions can be used to find and verify the characters for other point groups. For example, consider the partial character table for the point group C_{4v}.

A typical kind of exam or quiz question might be to fill in the missing values. In this case, all of the values are missing! So let's tackle the problem based on what we know from definitions, and complete the problem by using of the GOT.

C_{4v}	E	$2\ C_4$	C_2	$2\ \sigma_v$	$2\ \sigma_d$
A_1					
A_2					

C_{4v}	E	$2\,C_4$	C_2	$2\,\sigma_v$	$2\,\sigma_d$
B_1					
B_2					
E					

First off, the order of the group is $h = 8$. Second, every group has a totally symmetric representation. This is the A_1 representation and has members that are all 1. Let's fill that in (using red for clarity.)

C_{4v}	E	$2\,C_4$	C_2	$2\,\sigma_v$	$2\,\sigma_d$
A_1	1	1	1	1	1
A_2					
B_1					
B_2					
E					

Additionally, we can fill in the column for the identity element. All of the A and B representations are singly degenerate, and the E representation is doubly degenerate. So using the expression

$$\sum_i [\chi_i(E)]^2 = h$$

That yields the following (shown in *red*):

C_{4v}	E	$2\,C_4$	C_2	$2\,\sigma_v$	$2\,\sigma_d$
A_1	1	1	1	1	1
A_2	1				
B_1	1				
B_2	1				
E	2				

And it clearly satisfies

$$\begin{aligned} \sum_i [\chi_i(E)]^2 &= (1)^2 + (1)^1 + (1)^2 + (1)^1 + (2)^2 \\ &= 8 = h \end{aligned}$$

Now using the definition that A representations have a character of 1 for the (are symmetric with respect to) the principle rotation axis and B representations have a character of –1 for (or are antisymmetric with respect to) the principle axis rotation. Thus, we can fill in

C_{4v}	E	$2\,C_4$	C_2	$2\,\sigma_v$	$2\,\sigma_d$
A_1	1	1	1	1	1
A_2	1	1			
B_1	1	-1			
B_2	1	-1			
E	2	?			

But should we do about the character of the C_4 operation under the irreducible doubly degenerate representation E? One solution comes from another important consequence of the GOT. This can be stated as

$$\sum_i \chi_i(R_m)\chi_i(R_n) = h\delta_{mn}$$

Using this relationship, we can solve for the character of the C_4 operation under the E irreducible representation.

$$\begin{aligned} \textstyle\sum_i \chi_i(E)\chi_i(C_4) &= \textstyle\sum_i \chi_i(E)\left[2\chi_i(C_4)\right] \\ &= 2(1)(1)+2(1)(1)+2(1)(-1)+2(1)(-1)+2(2)x = 0 \end{aligned}$$

The only value of *x* that will satisfy this expression is *x* = 0. We can enter this value and also apply the definitions that the A_1 and B_1 representations are symmetric with respect to the σ_v operation and the A_2 and B_2 representations are antisymmetric with respect to σ_v.

C_{4v}	E	2 C_4	C_2	2 σ_v	2 σ_d
A_1	1	1	1	1	1
A_2	1	1		-1	
B_1	1	-1		1	
B_2	1	-1		-1	
E	2	0		?	

Again, the question mark can be removed as above.

$$\begin{aligned} \textstyle\sum_i \chi_i(E)\chi_i(\sigma_v) &= \textstyle\sum_i \chi_i(E)\left[2\chi_i(\sigma_v)\right] \\ &= 2(1)(1)+2(1)(-1)+2(1)(1)+2(1)(-1)+2(2)x = 0 \end{aligned}$$

Once again, as luck would have it, the only value of *x* that satisfies the equation is *x* = 0. Now, we can apply the GOT to the representations for A_1, and A_2 to generate an equation with two unknowns to determine the characters of C_2 and σ_d for representations A_2 and B_1. We can solve it because we know *x* and *y* can only be 1 or –1. (These are the only values possible for singly degenerate representations.)

$$\begin{aligned} \textstyle\sum_R \chi_i(R)\chi_j(R) &= \chi_1(E)\chi_2(E)+2\chi_1(C_4)\chi_2(C_4)+\cdots \\ &= (1)(1)+2(1)(1)+(1)x+2(1)(-1)+2(1)y = 0 \\ &= 1+x+2y = 0 \end{aligned}$$

C_{4v}	E	2 C_4	C_2	2 σ_v	2 σ_d
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1		1	
B_2	1	-1		-1	
E	2	0		0	

The only combination that works is $x = 1$ and $y = -1$. The character table now looks as follows:

Completion of the rest of the character table is left as an exercise.