

Construction of Character Table for C_{3v} Point Group

- (i) There are six symmetry operations present in C_{3v} point group i.e. $E, C_3^1, C_3^2, \sigma_a, \sigma_b, \sigma_c$.
 these operations are divide in the three classes i.e. $(E, 2C_3, 3\sigma_v)$ and hence there are three irreducible representations.

let they are $\Gamma_1, \Gamma_2, \Gamma_3$.

- (ii) The sum of the squares of dimensions (i.e. characters of the identity operation) should be equal to six (or 6).

$$\sum l_i^2 = l_1^2 + l_2^2 + l_3^2 = 6$$

The values of l_i that will satisfy this requirement are 1, 1, and 2.

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_1	1		
Γ_2	1		
Γ_3	2		

- (iii) Every point group possesses one representation which is totally symmetric.

In this representations, all the operations have the character value one (1).

Thus we have

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_1	1	1	1

It can be seen that the summation of the square of the character of the operations is equal to 6

$$1^2 + 2 \times 1^2 + 3 \times 1^2 = 6$$

- (iv) Γ_2 (Second irreducible representation), must be orthogonal to Γ_1 .
 since $\chi_2(E)$ must always be positive and hence Γ_2 must consist of three +1 and three -1. This is only possible if Γ_2 has 1, 1, and -1.

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	1	1	-1

(v) One third representations will be of two and hence $\chi_3(E)$ is 2.
 In order to find out the values of $\chi_3(C_3)$ and we make the use of the orthogonality relationship.
 Γ_1 and Γ_3 are orthogonal to each other
 Γ_2 and Γ_3 are also

C_{3v}	E	$2C_3$	$3C_2$
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	$\chi_3(C_3)$	$\chi_3(C_2)$

$$\sum_R \chi_1(R) \cdot \chi_3(R) = (1) \cdot (2) + 2(1) \cdot \chi_3(C_3) + 3 \cdot (1)$$

$$\text{and } \sum_R \chi_2(R) \cdot \chi_3(R) = (1) \cdot (2) + 2(1) \cdot \chi_3(C_3) + 3 \cdot (-1)$$

Solving equation (i) and (ii) we get

$$2\chi_3(C_3) + 3\chi_3(C_2) = -2$$

$$2\chi_3(C_3) - 3\chi_3(C_2) = -2$$

On adding eqⁿ (iii) and (iv) we get

$$4\chi_3(C_3) = -4$$

$$\therefore \chi_3(C_3) = -1$$

This value is substituted in equation (iii) to

$$2(-1) + 3\chi_3(C_2) = -2$$

$$3\chi_3(C_2) = 0$$

$$\chi_3(C_2) = 0$$

Thus, the complete set of characters of irreducible of C_{3v} point group is

C_{3v}	E	$2C_3$	$3C_2$
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

The complete character table for the point group C_{3v} is given as follows.

C_{3v}	E	$2C_3$	$3C_2$		
A_1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	(x, y) (R_x, R_y)	$(x^2 - y^2, xy)$ (xz, yz)
I		II		III	IV

In the upper left corner of the table is the Schoenflies notation for the group and the upper row of the table consists of the symmetry operations grouped in classes.

Area I represents the symbols for irreducible representations according to Mulliken.

Because first two irreducible representations are unidimensional and hence A or B may be used.

The character of principal axis of rotation for both the representations are symmetrical and hence A is used.

Subscript 1 is written for the symmetrical character (+1) of operation C_2 , while subscript 2 is written for unsymmetrical character (-1) of operation C_2 .

The symbol E shows the two dimensional representation.

Area II :- In area II of the table are the characters of the irreducible representation of the point groups.

Area III :- Area III gives the transformation properties of Cartesian co-ordinates x, y, z and rotation about x, y & z axes i.e. R_x, R_y and R_z .

Area IV :-

In this area IV of the table, squares and binary products of co-ordinates according to their transformation properties are described.

The squares of the vectors $(x^2 - y^2)$ and z^2 belong to A_1 , $x^2 - y^2$ and xy taken together and xz, yz taken together belong to E.