

## Mulliken Symbols for Various Irreducible Representations of a Point Group.

The symbols for irreducible representation were given by Mulliken, hence they are known as Mulliken Symbols.

### Rules.

These symbols can be found by the following

- (i) All unidimensional representations are represented either by A or B, two dimensional representations are represented by E, and three dimensional representations are represented by T.
- (ii) One dimensional representations which are symmetrical with respect to the principal axis (i.e. character of  $C_n$  operation is +1) are designated as A while those antisymmetric (in this respect (i.e. character of  $C_n$  operation -1)) are designated as B.
- (iii) Those irreducible representations which are symmetrical with respect to the subsidiary axis, or, in its absence to  $\sigma_v$  plane, subscript 1, (i.e.  $A_1, B_1, E_1, T_1$ ) is used and for antisymmetric subscript 2 (i.e.  $B_2, A_2, E_2, T_2$ ) is used.
- (iv) Primes and double primes are attached to all A, B, E or T to indicate the symmetric and antisymmetric character, with respect to  $\sigma_h$ ,  $A'$  or  $E'$  appears for  $\sigma_h$  having +1 and  $A''$  or  $E''$  appears for the  $\sigma_h$  having -1.

- (v) Subscript g and u are used to indicate the symmetric and antisymmetric character with respect to the inversion. If the point group has no centre of symmetry, g and u are not used. Term g stands for gerade (Centro Symmetric) and u stands for ungerade (Non-Centro Symmetric).

## Construction of character table for $C_{2v}$ Point group.

- (i) There are total number of four symmetry operations in  $C_{2v}$  point group  
i.e.  $E, C_{2(z)}, \sigma_{xy}, \sigma_{yz}$

- (ii) These operations belong to four different classes hence there are four irreducible representations let them be  $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$

(iii) It also requires that the sum of the square of the dimensions of these representations equals  $h$  (order of the group) i.e. 4.

Hence each representation must be unidimensional  
 so that  $1^2 + 1^2 + 1^2 + 1^2 = 4$

Because the character of identity operation is equal to the dimension of the representation and hence  $\chi$  must be equal to one (1) in all of them.

	E	$C_2(z)$	$\sigma_{xz}$	$\sigma_{yz}$
$\Gamma_1$	1			
$\Gamma_2$	1			
$\Gamma_3$	1			
$\Gamma_4$	1			

The sum of the squares of the character of an irreducible representation must be equal to 4 as

$$\sum_R [\chi_i(R)]^2 = 4$$

i.e.  $1^2 + 1^2 + 1^2 + 1^2 = 4$

	E	$C_2(z)$	$\sigma_{xz}$	$\sigma_{yz}$
$\Gamma_1$	1	1	1	1
$\Gamma_2$	1			
$\Gamma_3$	1			
$\Gamma_4$	1			

(iv) The sum of the squares of the characters of other irreducible representations must be equal to four and the character must also be orthogonal. Hence, character must include two +1 and two -1.

Hence character must include two +1 and two -1.  
 Therefore we will have,

	E	$C_2(z)$	$\sigma_{xz}$	$\sigma_{yz}$
$\Gamma$	1	1	1	1
$\Gamma$	1	-1	-1	1
$\Gamma$	1	-1	1	-1
$\Gamma$	1	1	-1	-1

All these representations are also orthogonal to one another taking  $\Gamma_2, \Gamma_3$  we have

$$(1)(1) + (-1)(-1) + (-1)(1) + (1)(-1) = 0$$