

**Q. What is the meaning of  $E'$  mulliken symbol?**

**Ans.** This is 2 dimensional irreducible representation which is Antisymmetric w.r.t. P-axis

Symmetric w.r.t. inversion

Symmetric w.r.t.  $\sigma_h$  in the molecule.

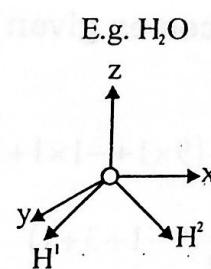
**Column II :**

II<sup>nd</sup> column of character table shows irreducible representation of the groups which can be derived using G.O.T.

**Column III :**

III<sup>rd</sup> column explain transformation properties of 3 cartesian coordinate x,y, z and 3 rotational axis i.e.  $R_x, R_y, R_z$ .

$C_{2v}$	E	$C_2$	$\sigma_{xz}$	$\sigma_{yz}$	
x	1	-1	1	-1	$B_1$
y	1	-1	-1	1	$B_2$
z	1	1	1	1	$A_1$
$R_x$	1	-1	-1	1	$B_2$
$R_y$	1	-1	1	-1	$B_1$
$R_z$	1	+1	-1	-1	$A_2$



**Column IV :**

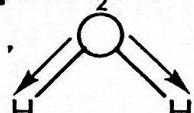
IV<sup>th</sup> column explain transformation properties of quadratic functions of cartesian coordinates like transformation properties of  $x^2, y^2, z^2$ .

$$x^2 - y^2, xy, yz, xz, x^2 - y^2 - z^2$$

$C_{2v}$	E	$C_2$	$\sigma_{xz}$	$\sigma_{yz}$	
x	1	-1	1	-1	
y	0	-1	-1	1	
z	1	1	1	1	
$x^2, y^2, z^2$	0	1	1	1	$A_1$
$xz$	1	-1	1	-1	$B_1$
$yz$	1	-1	-1	1	$B_2$
$xy$	1	1	-1	-1	$A_2$

$C_{2v}$	E	$C_2$	$\sigma_{xz}$	$\sigma_{yz}$
$A_1$	1	1	1	1
$A_2$	1	1	-1	-1
$B_1$	1	-1	1	-1
$B_2$	1	-1	-1	1

**Example:  $H_2O$  :**

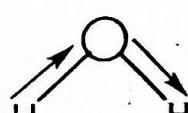


$C_2 \checkmark$

$\sigma_{xz}$

$\sigma_{yz} \checkmark$

$A_1$  vibration

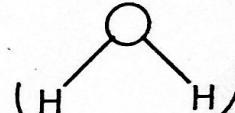


$C_2 \times$

$\sigma_{xz} \checkmark$

$\sigma_{yz} \times$

$B_1$  vibration



$C_2 \checkmark$

$\sigma_{xz} \checkmark$

$\sigma_{yz} \checkmark$

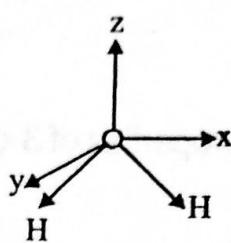
$A_1$  vibration

**RELATION BETWEEN REDUC-**

$A_1$  &  $B_1$  vibrations are I.R. active.

**Reduction of a reducible representation : conversion of a higher dimension to a lower dimension representation.**

$C_{2v}$	E	$C_2$	$\sigma_{xy}$	$\sigma_{yz}$
R.R.	9	-1	3	1



$C_{2v}$	E	$C_2$	$\sigma_{xy}$	$\sigma_{yz}$
$A_1$	1	1	1	1
$A_2$	1	1	-1	-1
$B_1$	1	-1	1	-1
$B_2$	1	-1	-1	1

**Q. How many times  $A_1$  comes given by the formula?**

$$n_{A_1} = \frac{1}{4}(9 \times 1 + -1 \times 1 + 3 \times 1 + 1 \times 1)$$

$$n_{A_1} = \frac{1}{4}(9 - 1 + 3 + 1)$$

$$n_{A_1} = \frac{12}{4}$$

$$n_{A_1} = 3$$

**Check :** Number comes always a complete no.

$$n_{A_2} = \frac{1}{4}(9 \times 1 + -1 \times 1 + 3 \times -1 + 1 \times -1)$$

$$n_{A_2} = \frac{1}{4}(9 - 1 - 3 - 1)$$

$$n_{A_2} = \frac{4}{4} = 1$$

$$n_{A_2} = 1$$

$$n_{B_1} = \frac{1}{4}(9 \times 1 + -1 \times -1 + 3 \times 1 + 1 \times -1)$$

$$= \frac{1}{4}(9 + 1 + 3 - 1)$$

$$= \frac{12}{4} = 3$$

$$n_{B_1} = 3$$

$$n_{B_2} = \frac{1}{4}(9 \times 1 + -1 \times -1 + -1 \times 3 + 1 \times 1)$$

$$n_{B_2} = \frac{1}{4}(9 + 1 - 3 + 1)$$

$$n_{B_2} = 2$$

then  $3A_1 + 1A_2 + 3B_1 + 2B_2$

it is count the dimension = 9

$$n_{T_1} = \frac{1}{24} [(4 \times 3) + 8(1 \times 0) + 3(0 \times -1) + 6(0 \times +1) + 6(2 \times -1)]$$

$$n_{T_1} = \frac{1}{24} (12 + 0 + 0 + 0 - 12)$$

$$n_{T_1} = \frac{0}{24}$$

$$n_{T_1} = 0$$

$$n_{T_2} = \frac{1}{24} [4 \times 3 + 8(1 \times 0) + 3(0 \times -1) + 6(0 \times -1) + 6(2 \times 1)]$$

$$n_{T_2} = \frac{1}{24} (12 + 0 + 0 + 0 + 12)$$

$$n_{T_2} = \frac{24}{24} = 1$$

$$n_{T_2} = 1$$

So  $A_1 + T_1$

For Recheck :

$A_1$	1	1	1	1	1
$T_1$	1	1	-1	1	-1
R.R.	4	1	0	2	0
Total					