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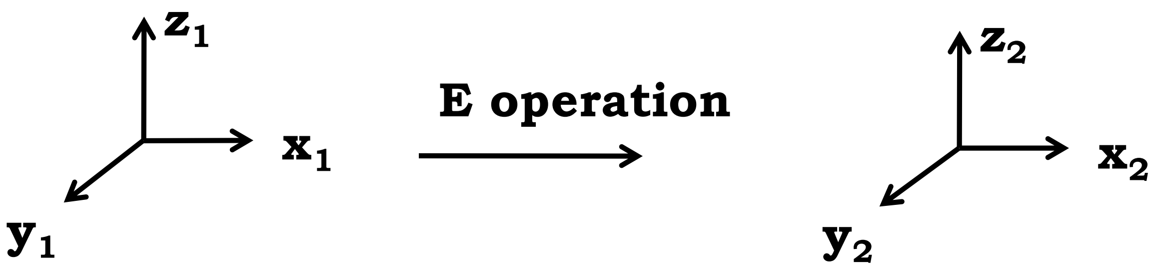
- Representation of Group by Matrix
- Group multiplication table
- Rule for construction of Character Table
- Mulliken symbol

Representation of Group by Matrix : Various symmetry operations like E, σ, i, $C_{n(z)}$ and $S_{n(z)}$ can be represented by matrix

Identity matrix (E) : coordinate (x,y,z) of object



No change of sign of coordinate after E operation,

$$(x_1, y_1, z_1) \xrightarrow{\text{E operation}} (x_2, y_2, z_2)$$

it can be represented in the form of equation

$$x_2 = x_1$$

$$y_2 = y_1$$

$$z_2 = z_1$$

$$x_2 = 1.x_1 + 0.y_1 + 0.z_1$$

$$y_2 = 0.x_1 + 1.y_1 + 0.z_1$$

$$z_2 = 0.x_1 + 0.y_1 + 1.z_1$$

it can be represented in the form of matrix

$$\begin{vmatrix} x_2 \\ y_2 \\ z_2 \end{vmatrix} \begin{matrix} = \\ = \\ = \end{matrix} \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{vmatrix} . \begin{vmatrix} x_1 \\ y_1 \\ z_1 \end{vmatrix}$$

$$E = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

Similarly

Matrix for σ_{xy} plane

$$\sigma_{xy} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{vmatrix}$$

Matrix for σ_{yz} plane

$$\sigma_{XZ} = \begin{vmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

Matrix for σ_{xz} plane

$$\sigma_{XZ} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

Matrix for (i) inversion operation

$$i = \begin{vmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{vmatrix}$$

Matrix for $Cn_{(z)}$ rotation operation

$$C_{n(Z)} = \begin{vmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

θ	60°	90°	120°	180°
$\sin\theta$	√3/2	1	√3/2	0
$\cos\theta$	1/2	0	- 1/2	-1

θ - angle of rotation

Q1. Find the matrix representation of C_2, C_3 & C_4 operations.

Matrix for $S_{n(z)}$ rotation operation

$$S_{n(Z)} = \begin{vmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & -1 \end{vmatrix}$$

θ	60°	90°	120°	180°
$\sin\theta$	$\sqrt{3}/2$	1	$\sqrt{3}/2$	0
$\cos\theta$	1/2	0	- 1/2	-1

Q1. Find the matrix representation of S_2, & S_4 operations.

Group multiplication table : Product of symmetry operation can be compiled in the form of table is called Group multiplication table

Q1. Prepare the group multiplication table for C_3 point group

C_3	E	$C^1{}_3$	$C^2{}_3$
E			
$C_3{}^1$			
$C_3{}^2$			

$$C_n{}^m \,.\, C_n{}^k = C_n{}^{(m+k)}$$

Q2. Prepare the group multiplication table for C_4 point group

C_4	E	$C^1{}_4$	$C^2{}_4$	$C^3{}_4$
E				
$C_4{}^1$				
$C_4{}^2$				
$C_4{}^3$				

Q3. Prepare the group multiplication table for C_{2v} point group

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
E				
C_2				
σ_{xz}				
σ_{yz}				

Use matrix of E, C_2 , σ_{xz} and σ_{yz} for finding the product of symmetry operation

Q4. Prepare the group multiplication table for C_{2h} point group

$\mathbf{C_{2h}}$	E	C_2	σ_{xy}	i
E				
C_2				
σ_{xy}				
i				

Character Table :It is a description of character under each class for irreducible representations

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	-1	1
Γ_4	1	-1	1	- 1

Rule for construction of Character Table

Rule 1: Let E, A, B, , C, be the nonequivalent element of symmetry operation that can be carried out on the molecule , It should be written upper side of the table,

C_{2V}	E	C_2	σ_{xz}	σ_{yz}

Rule 2: Let Γ_1,Γ_2, Γ_3 & Γ_4 be the nonequivalent irreducible representation, which is equal to order of group, It should be written Left side in the column of the table.

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1				
Γ_2				
Γ_3				
Γ_4				

Rule3: Let ℓ_1, ℓ_2, ℓ_3 & ℓ_4 be the dimension irreducible representation. The Sum of the square of the dimension is equal to order of group,

$$\ell^2_1 + \ell^2_2 + \ell^2_3 + \ell^2_4 = h$$

$$\sum l^2_i = h$$

calculated values are written under E class.

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1				
Γ_2				
Γ_3				
Γ_4				

Rule4: Let $g(R)$ be the multiplying factor of each classes and $\chi_i(R)$ be the irreducible representation under each classes then the

$$\sum g(R)[\chi_i(R)]^2 = h$$

Rule5: Orthogonality rule : Let $g(R)$, be the multiplying factor of each classes & $\chi_i(R)$ & $\chi_j(R)$ be the character of irreducible representation under each classes then the

$$\Gamma_i . \Gamma_j = \sum g(R)[\chi_i(R)]\,[\chi_j(R)] = 0$$

Q. 1. Construct the character table for C_{2v} point group using suitable rules

C2v= (E, C_2, σ_{xz}, , σ_{yz},) , Order of group= 4

According to Rule 1: Let E, C_2, σ_{xz}, , σ_{yz}, be the element of symmetry operation that can be carried out on water molecule, It should be written upper side of the table,

C_{2V}	E	C_2	σ_{xz}	σ_{yz}

According to Rule 2: Let Γ_1,Γ_2, Γ_3 & Γ_4 be the nonequivalent irreducible representation, which is equal to order of group, It should be written Left side in the column of the table.

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1				
Γ_2				
Γ_3				
Γ_4				

According to Rule3: Let ℓ_1, ℓ_2, ℓ_3 & ℓ_4 be the dimension irreducible representation. The Sum of the square of the dimension is equal to order of group,

$$\sum l^2_i = h$$

calculated values are written under E class.

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1	1			
Γ_2	1			
Γ_3	1			
Γ_4	1			

$$\sum \ell^2_i = h$$

$$\ell^2_1, + \ell^2_2 + \ell^2_3 + \ell^2_4 = 4$$

$$1^2 + 1^2 + 1^2 + 1^2 = 4$$

According to Rule4: Let g(R) be the multiplying factor of each classes and $\chi_i(R)$ be the irreducible representation under each classes then the

$$\sum g(R)[\chi_i(R)]^2 = h$$

$$g(E)[\chi_1(E)]^2 + g(C_2)[\chi_1(C_2)]^2 + g(\sigma_{xz})[\chi_1(\sigma_{xz})]^2 + g(\sigma_{yz})[\chi_1(\sigma_{yz})]^2 = h$$

$$: 1x[1]^2 + 1x[\chi_1(C_2)]^2 + 1x[\chi_1(\sigma_{xz})]^2 + 1x[\chi 1(\sigma_{yz})]^2 = 4$$

$$: 1x[1]^2 + 1x[1]^2 + 1x[1)]^2 + 1x[1]^2 = 4$$

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1	1	1	1	1
Γ_2	1			
Γ_3	1			
Γ_4	1			

According to Orthogonality rule : Let g(R), be the multiplying factor of each classes $\chi_i(R)$ & $\chi_j(R)$ be the character of irreducible representation under each classes then the

$$\Gamma_i . \Gamma_j = \sum g(R)[\chi_i(R)]\,[\chi_j(R)] = 0$$

$$\begin{aligned}\Gamma_1 . \Gamma_2 = {} & g(E)\times[\chi_1(E)]\times[\chi_2(E)] \\ & + g(C_2)\times[\chi_1(C_2)]\times[\chi_2(C_2)] \\ & + g(\sigma_{xz})\times[\chi_1(\sigma_{xz})]\times[\chi_2(\sigma_{xz})] \\ & + g(\sigma_{yz})\times[\chi_1(\sigma_{yz})]\times[\chi_2(\sigma_{yz})] = 0\end{aligned}$$

$$\begin{aligned}\Gamma_1 . \Gamma_2 = {} & 1\times1\times1 \\ & + 1\times1\times[\chi_2(C_2)] \\ & + 1\times1\times[\chi_2(\sigma_{xz})] \\ & + 1\times1\times[\chi_2(\sigma_{yz})] = 0\end{aligned}$$

Any two characters are negative

$$\begin{aligned}\Gamma_1 . \Gamma_2 = {} & 1\times1\times1 + 1\times1\times[1] \\ & + 1\times1\times[-1] + 1\times1\times[-1] = 0\end{aligned}$$

$$\Gamma_1 . \Gamma_2 = 1 + 1 - 1 - 1 = 0$$

$$\Gamma_2 = (1, 1, -1, -1)$$

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1			
Γ_4	1			

Similarly way the Γ_2. Γ_3 orthogonal to each other then the characters of Γ_3=(1,-1-1 , 1)

And Γ_2. Γ_4 orthogonal to each other then the characters of Γ_4=(1,-1, 1 , -1)

C_{2V}	E	C_2	σ_{xz}	σ_{yz}
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	-1	1
Γ_4	1	-1	1	-1

Q. 1. Construct the character table for C_{3v} point group using suitable rules

$C_{3v} = \{E, 2C_3, 3\sigma v\}$ order of group (h)= 6

According to Rule 1, $E, 2C_3, 3\sigma_v$ irreducible representation

According to Rule 2 : Let $\Gamma_{1,} \Gamma_{2}, \Gamma_{3}$ irreducible representation

According to Rule 3 , $\sum l^2_i = h$

According to rule 4, $\sum g(R)[\chi_i(R)]^2 = h$

C_{3V}	E	$2C_2$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	1		
Γ_3	2		

According to orthogonality rule $\Gamma_i . \Gamma_j = \sum g(R)[\chi_i(R)][\chi_j(R)] = 0$

Γ_1 Γ_2 are orthogonal to each other , we get

C_{3V}	E	$2C_2$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2		

Γ_1 and Γ_2 are orthogonal to each other ; Γ_1 and Γ_3 are orthogonal to each other

Apply $\Gamma_1 \Gamma_2 = \sum g(R)[\chi_i(R)][\chi_j(R)] = 0$ $\Gamma_1 \Gamma_3 = \sum g(R)[\chi_i(R)][\chi_j(R)] = 0$

C_{3V}	E	$2C_2$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	x	y

Find the values x & y by solving simultaneous equation

Q1. find the dimension of $\Gamma_{1,} \Gamma_{2,} \Gamma_{3,} \Gamma_{4,} \Gamma_5$ irreducible representation in the following character table using suitable rule

T_d	E	$6C_4$	$3C_2$	$6S_4$	$6\sigma_d$
Γ_1					
Γ_2					
Γ_3					
Γ_4					
Γ_5					

Q2. find the character under E class of following character table

D_3	E	$2C_3$	$3C_2$
Γ_1			
Γ_2			
Γ_3			

Q3. find character of Γ_1 under each classes of following character table.

T_d	E	$6C_4$	$3C_2$	$6S_4$	$6\sigma_d$
Γ_1					

THE END