

Point gr | (B)

C_{2v} linear molecule
HCl, CO, C₂H₂
Asymmetric

(1) C_{nh} point gr $\rightarrow$

formula $C_{nh} = C_n + 1\sigma_h$

Total No of elements / operation = $2n$

(2) C_{nv} point gr $\rightarrow$

$$C_{nv} = C_n + n\sigma_v$$

(as $C_{3v} = NH_3$)

Total No of operations = $(2n)$

As if $n=2$, then $C_{2v} = 4 = \underset{(1)}{C_2} + \underset{(2)}{2\sigma_v} + \underset{(1)}{E}$

(3) D_{nh} point gr $\rightarrow$

formula $\rightarrow C_n + nC_2 + n\sigma_v + 1\sigma_h$

No. of operation = $(4n)$

As if $(n=2)$ then $\rightarrow$

$$8 = D_{2h} = \underset{(1)}{C_2} + \underset{(2)}{2C_2} + \underset{(2)}{2\sigma_v} + \underset{(1)}{1\sigma_h} + \underset{(1)}{E} + \underset{(1)}{S_2}$$

$[D_{2h} = CO_2]$

as $[BF_3 \rightarrow D_{3h}]$

$$\rightarrow C_3 + 3\sigma_v + 1\sigma_h + 3C_2$$

(4) D_{nd} point gr $\rightarrow C_n + nC_2 + n\sigma_d$

No of operations = $(4n)$

As $\rightarrow 8 = D_{2d} = \underset{(1)}{C_2} + \underset{(2)}{2C_2} + \underset{(2)}{2\sigma_d} + \underset{(1)}{E} + \underset{(2)}{S_4}$

⑤ C_n point gr $\rightarrow$ $C_n + E$
no of operations = n

as $C_2 = C_2 + E$
 $C_3 = C_3 + E$

⑥ S_{2n} point gr
 $\rightarrow S_{2n} + C_n + E$
 $\rightarrow$ no of operation = $2n$
 $\rightarrow$ as $S_4 = S_4 + C_2 + E$
② ① ① = 4

⑦ D_n point gr $\rightarrow$
 $C_n + nC_2$
 $\rightarrow$ no of operations = $2n$

as $6 = D_3 = C_3 + 3C_2 + E$
② ③ ①

Each molecular point gr में matrix representation 2 तरीके से करते हैं

- ① Irreducible → ये character (x) हैं
- ② Reducible

→ एक molecular point gr में जितने class (symmetry elements) होंगे, उतने ही character & irreducible representation होंगे।

as E का matrix representation ये है →

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow \text{इसमें upper left से lower right में चलने पर जो elements होते उनके addition को ही character}$$

↓

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \xrightarrow{\text{Block method से,}} \text{E के irreducible representation होंगे } 1, 1, 1$$

$$C_2 \rightarrow \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow -1 \quad -1 \quad 1$$

$$\sigma_{xz} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow 1 \quad -1 \quad 1$$

$$\sigma_{yz} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = -1 \quad 1 \quad 1$$

→ किसी भी molecular point gr में उतने ही character होंगे, जितने class (symmetry element) होंगे

1/2/19

(10) as C_{2v} point gr में 4 class

हैं, so 4 character होंगे।

(C_{2v}) → block method में प्राप्त value लिख लेते हैं

	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				

→ ये एक type का representation

ये IE की 4 value हो सकती हैं उनमें से $\Gamma_1, \Gamma_2, \Gamma_3$ को एक block method (Matrix) में निकाल सकते हैं & चौथी value को Group Theorem से निकालते हैं

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(11)

Reducible

Matrix representation
(2 तरीकों से)

(Decomposed)

बहुत लम्बी Matrix
को छोटे-2 block में
represent करते हैं

(Reduced)

जब छोटे-2 block
को दाव और आगे
छोटे-2 part में
न हो सकते हैं

Order = NO of symmetry elements

(14)

Rule No 4 → The character of symmetry operation

[GOT] Theorem (12)

If $\Gamma_1, \Gamma_2, \Gamma_3 \rightarrow$ irreducible representations
 $l_1, l_2, l_3 \rightarrow$ dimensions

① The NO of irreducible representations in a gr = NO of classes in the group.

C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$
Γ_1				
Γ_2				
Γ_3				
Γ_3				

Where $E, C_2(z), \sigma_v(xz)$ & $\sigma_v(yz)$ are 4 classes of C_{2v} point gr

(2)

(15)

one operation associated

	C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$
Γ_1	1	1	1	1	1
Γ_2	1	1	-1	-1	1
Γ_3	1	1	-1	1	-1
Γ_4	1	1	1	1	-1

There are different irreducible representations

Rule II → The sum of squares of characters of the identity operations in the irreducible is equal to h

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

$$1^2 + 1^2 + 1^2 + 1^2 = (4)$$

of this character table
Order_n = (4)

Rule III → The sum of squares of dimensions of the irreps of a group is equal to h

$$\sum_{l=0}^K l^2 = h$$

i.e. each element $\vec{h}$ has one operation associated with it. Each $\vec{h}$ has one $\vec{h}$.
 So, our table is C_{2v} point group. Each $\vec{h}$ dimension one. So $1^2 + 1^2 + 1^2 + 1^2 = (4)$

order = no of symmetry elements

(14)

Rule No 4 → The characters of symmetry operations in two different irreps are orthogonal to each other

$$\sum [g_p \chi_i(R) \chi_j(R)] = 0$$

(g_p = 1) $\begin{matrix} & & C_2 & & \sigma_v \\ E & & & & \end{matrix}$

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

(5) The characters of all the matrices belonging to the symmetry operations in the same class are identical

~~(3, 1, 3, 2, 4) irreps~~
~~(4, 1, 2, 2, 2) symmetry operations~~

C_{2v} point gr $\frac{8}{h}$ each class or symmetry operation is
 element $\frac{8}{24}$ of symmetry operation $\frac{8}{24}$
 so (g_p = 1)

GOT theory