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- Mulliken symbolism Rules for Irreducible representation
- Direct product of irreducible representation
- Standard reduction formula

Mulliken symbol .

A, B, E, T , A_g, A_{1g}, A_{2g}, B_g, B_{1g},B_{2g}, A_u, B_u, E, E_g, T_{1g}, T_{2g} T_{2u}

What are a meaning of Mulliken symbols ?

1 dimension = A or B
2 dimension = E
3 dimension = T

Dimension of irreducible subscript

$\mathbf{B_{1u}}$

T_{2g}

Alphabetical subscript

See the character under i or σ_h

Symmetric – lable g

+ sign

Asymmetric label u

- sign

Numerical subscript

See the character under Subsidiary axis or σ_v

- Sign - Asymmetric label 2

Mulliken symbolism Rules for Irreducible representation .

❖ Consider character table for C_{3v} point group .

C_{3V}	E	$2C_2$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

❖ A_1, A_2, E be the Mulliken symbol which has certain meaning

See the character under E class and represent symbol A, B, E and T using following rule.

1. Dimensionality Rule :

All one dimensional representation s are designated by either A or B symbol

Two dimensional IRs representation n is designated by E

Three dimensional IRs representation n is designated by T

2. See the character under Principle axis for labeling one dimensional A & B

if $\chi(C_n) = +1$ ----------- symmetric representation --- label A

if $\chi(C_n) = -1$ ----------- asymmetric representation --- label B

3. Numerical Subscript rule : 1 &2 numerical subscript are attached A , B, T representation for that see the character under secondary axis C_2

if $\chi(C_2) = +1$ ----------- symmetric representation --- label '1'

if $\chi(C_2) = -1$ ----------- asymmetric representation --- label '2'

if Secondary axis is absent then see the character under vertical plane

if $\chi(\sigma_v) = +1$ ----------- symmetric representation --- label "1"

if $\chi(\sigma_v) = -1$ ----------- asymmetric representation --- label "2'

4. Alphabetical subscript rule : g &u subscript are attached to A , B, T representation for that see the character under center of inversion (i) class

if $\chi(i) = +1$ ----------- symmetric representation --- label 'g 'subscript

if $\chi(i) = -1$ ----------- asymmetric representation --- label 'u' subscript

Question1 : Transform the $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$ into Mulliken symbols of the following character table

Ex: 1

C_{3V}	E	$2C_3$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

Ex: 2

C_{2h}	E	C_2	i	σ_h
Γ_1	1	1	1	1
Γ_2	1	-1	1	-1
Γ_3	1	1	-1	-1
Γ_4	1	-1	-1	1

Direct product of irreducible representation :

C_{2V}	E	C_2	σ_{xz}	σ_{yz}	Direct product
A_1	1	1	1	1	
A_2	1	1	-1	-1	
B_1	1	-1	-1	1	
B_2	1	-1	1	-1	
$A_1 x A_2$	1	1	-1	-1	A_2
$A_2 x A_2$	1	1	1	1	A_1
$A_2 x B_1$	1	-1	1	-1	?

Product of Dimension : A, B, E, T
AxA= A, BxB =A
AxB =BxA= B
AxE =BxE =E
ExE =A+T or B +T depend on P. G
ExT = A+E+T
TxT = A +E+T +T

Product of subscript : 1,2,g,u
1x1= 1 gxg=g
1x2= 1 gxu=u
2x2= 1 uxu=g

[symmetric]x[symmetri] = symmetric

[symmetric]x[asymmetri] = asymmetric

[asymmetric]x[asymmetric] = symmetric

Standard reduction formula :

$$n(\Gamma_i) = [g(R).\chi_{IR}(R).\,\boldsymbol{\chi_{RR}(R)}\,]/h$$

Where

g(R) - multiplying factor of respective class

χ_{IR} (R). – character if IRs representation under respective class

χ_{RR} (R - character if RRs representation under respective class

h- order of group

Q1. Find out number of time A_1, A_2, B_1, and B_2 will appear in the following table order of group

C_{2V}	E	C_2	σ_{xz}	σ_{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
$\boldsymbol{\chi_{RR}}$ **(R)**	15	-1	3	3

Q1. Find out number of time A_1, A_2, E will appear in the following table order of group

C_{3V}	E	$2C_3$	$3\sigma_v$
A1	1	1	1
A2	1	1	-1
E	2	-1	0
χ_{RR} **(R)**	21	0	3

THE END