(5) * Construct the character table of C_{3v} (NH_3) point Group :—

It is conveniently deduced from the consequence of Orthogonality theorem. There are three classes in C_{3v} - point Group.
viz. E, $2C_3$ & $3\sigma_v$.

~~A/c to Orthogo~~ Sum ~~some~~ of the square of character of identity operation representating dimension of the group, which corresponds to the order of the group. As there are three class so, we aspect three Irreducible representation. Viz. Γ_1, Γ_2 & Γ_3 respectively.

There is another property, the sum of the square of various symmetry operation multiplyed by no. of class in each case also is equal to the order of the group. (h).

In C_{3v}-point group order is taken to be six (6).

Hence,

$$g_1\{\chi(E)\}^2 + g_2\{\chi(C_3)\}^2 + g_3\{\chi(\sigma_v)\}^2 = 6.$$

where, g_1, g_2 & g_3 are the order of the classes for E, C_3 & σ_v respectively.

So,

$$1\times1^2 + 2\times1^2 + 3\times1^2 = 6$$

$$1 + 2 + 3 = 6$$

$$LHS = RHS$$

So, the character of M_1 will be always totally symmetric (i.e 1, 1, 1)

$\therefore M_1 = 1 \quad 1 \quad 1$

C_{3v}	E	$2C_3$	$3\sigma_v$
M_1	1	1	1

The other property is applied here —
sum of the square of the character of identity is equal to the order of the group.

Thus –

$$1^2 + 1^2 + 2^2 = 6$$

$$1 \quad 1 + 4 = 6$$

Thus the character of E will be –

	E	$2C_3$	$3\sigma_v$
M_1	1		
M_2	1		
M_3	2		

The character of other symmetry operation may be labbeled a & b corresponding to M_2 and c&d Corresponding to M_3.

Thus –

C_{3v}	E	$2C_3$	$3\sigma_v$
M_1	1	1	1
M_2	1	a	b
M_3	2	c	d

On applying Orthogonality condition between Γ_1 & Γ_2.

$$g_1 \chi_1(E) \cdot \chi_2(E) + g_2 \chi_1(C_3) \cdot \chi_2(C_3) + g_3 \chi_1(\sigma_v) \cdot \chi_2(\sigma_v) = 0$$

Here g_1, g_2 & g_3 is 1, 2 & 3 respectively.

$$1 \times 1 \times 1 + 2 \times 1 \times a + 3 \times 1 \times b = 0$$

or $1 + 2a + 3b = 0$ or $2a + 3b = -1$ —— (1)

we discuss previously, the sum of the square of various symmetry operation multiplied by no. of class is equal to the order of the group (h)

$$\therefore \quad 1^2 + 2a^2 + 3b^2 = 6$$

$$1 + 2a^2 + 3b^2 = 6 \quad \text{—— (2)}$$

Since, $2a + 3b = -1$

$$2a = -(3b+1)$$

$$a = -\tfrac{1}{2}(3b+1) \quad \text{—— (3)}$$

from eqn —(2)

$$2a^2 + 3b^2 = 6 - 1$$

$$2a^2 + 3b^2 = 5 \quad \text{—— (4)}$$

putting the value of a from -(3) into (4) we get-

$$\cancel{2} \times \frac{1}{\cancel{4}\,2}(3b+1)^2 + 3b^2 = 5$$

$$\left[\frac{(3b+1)^2}{2} + \frac{3b^2}{1} = 5\right.$$

$$\frac{(3b+1)^2 + 6b^2}{2} = 5$$

$$(3b+1)^2 + 6b^2 = 10$$

or $\frac{1}{2}(3b+1)^2 + 3b^2 = 5$

or $(3b+1)^2 + 6b^2 = 10$

$9b^2 + 2 \times 3b \times 1 + (1)^2 + 6b^2 = 10$

or $9b^2 + 6b + 1 + 6b^2 = 10$

$15b^2 + 6b + 1 = 10$

or $15b^2 + 6b = 9$

or $15b^2 + 6b - 9 = 0$

$3(5b^2 + 2b - 3) = 0$

or $5b^2 + 2b - 3 = 0$

or $5b^2 + 5b - 3b - 3 = 0$

$5b(b+1) - 3(b+1) = 0$

$(5b-3)(b+1) = 0$

$5b-3 = 0$	$(b+1) = 0$
$5b = 3$	$b = -1$
$b = 3/5$	

$3/5$ is a fraction. Hence, it is unacceptable.

Thus

we have $\boxed{b = -1}$

Now putting the value of b in eq^n - 3 we get -

$$a = -\frac{1}{2}[3 \times (-1) + 1]$$

$$a = \frac{-1(-3+1)}{2}$$

$$a = \frac{-1(-2)}{2} = \frac{2}{2} = 1$$

$\therefore \boxed{a = 1}$

Similarly,
we can deal with Γ_1 & Γ_3 on using orthogonality condition -

$$g_1 \chi_1(E)\cdot\chi_3(E) + g_2\chi_1(C_3)\cdot\chi_3(C_3) + g_3\chi_1(\sigma_v)\cdot\chi_3(\sigma_v) = 0$$

here g_1, g_2 & g_3 are 1, 2, 3 respectively.
Thus -

$$1\times1\times2 + 2\times1\times c + 3\times1\times d = 0$$
$$2 + 2c + 3d = 0 \text{ or } 2c+3d = -2 \quad \text{--- (5)}$$

The sum of the square of various symmetry operation multiplied by no. of class is equal to the order of the group (h).

$$\therefore 2^2 + 2c^2 + 3d^2 = 6$$
$$4 + 2c^2 + 3d^2 = 6 \quad \text{--- (6)}$$

Since,

$$2c + 3d = -2$$
$$2c = -(3d+2)$$

or

$$c = \frac{-(3d+2)}{2} \quad \text{--- (7)}$$

From eqn - (6)

$$2c^2 + 3d^2 = 2 \quad \text{--- (8)}$$

putting the value of (7) in eqn - (8) we get -

$$\cancel{2}\times\frac{(3d+2)^2}{\cancel{4}\,2} + 3d^2 = 2$$

$$\cancel{2\times\frac{9d^2+12d+4}{4} + 6d^2 = 6}$$

$$\cancel{2\times(9d^2+12d+4+6d^2)=6-4}$$
$$\cancel{9d^2+12d+4+6d^2=2}$$

or, $(3d+2)^2+6d^2=2\times2$

or, $9d^2+2\times3d\times2+4+6d^2=2\times2$

or, $15d^2+12d+4=2$

or, $15d^2+12d=0$

or, $3(5d^2+4d)=0$

or, $5d^2+4d=0$

or, $d(5d+4)=0$

$\therefore d=0$

$5d+4=0$

$d=-4/5$

$-4/5$ is a fractional. Hence, it is unaccepatable.

$\therefore \boxed{d=0}$

Now putting the value of 'd' in eqn (7) we get –

$$c=\frac{-(3\times0+2)}{2}$$

or, $c=\frac{-(0+2)}{2}$

or, $c=\frac{-2}{2}=-1$

$\therefore \boxed{c=-1}$

Thus, the character table

of C_{3v} - point group may be deduced as follows -

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

* Γ_1 & Γ_2 may be A or B. Γ_3 will be E

1st two are one dimensional representation.
The 3rd one is two " "

* Mülliken Notation :— (C_{3v})

(i) ~~character~~ Principal axis is C_3.
→ In first two cases, it is +ve [i.e. $\chi(C_3) = +1$]
Thus these two are assign to be 'A'
The character of C_3 for Γ_3 is immaterial.
It is two dimensional & assign to be E.

(ii) σ_v is present.
→ If character of σ_v is +ve
it is assign to be A_1 (subscript '1' is used).
→ If character of σ_v is -ve
it is assign to be A_2 (subscript '2' is used).
→ character of σ_v for Γ_3 is zero. So, it is of no matter.

So, Mülliken notations are → A_1, A_2 & E.

Thus, the character table of C_{3v}-point group with Mülliken notation may be constructed as follows —

C_{3v} → / MN ↓	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0