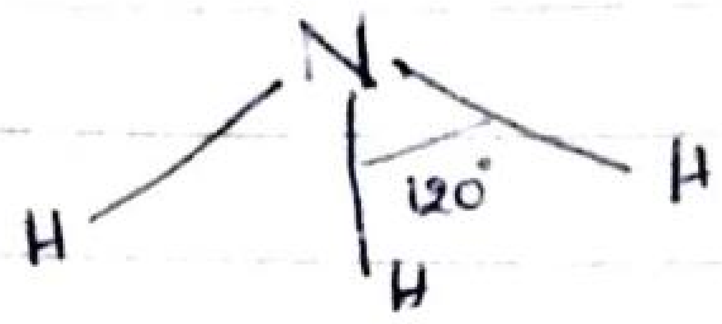
P.G. Sem. II^{nd} ; Inorg. Chem.

Core course VI

Unit IV

Multiplication table for C_{3v} group:- (e.g. NH_3)



Elements are :→

E, C_3^1, C_3^2, $\sigma_1(xz)$ or σ', σ_2 or σ'', σ_3 or σ'''.

No. of classes = 3.

∴ No. of I.R's. or symm. species = 3

Matrix representation of operations :—

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

$$C_3^1 = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$(\theta = 120^\circ)$

$\sin^+$	All +
$\tan^+$	$\cos^+$

$$= \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

$$C_3^2 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$(\theta = 240^\circ)$

$$\sigma_1 \text{ or } \sigma'(xz) = \begin{pmatrix} \cos 2\alpha & \sin 2\alpha & 0 \\ \sin 2\alpha & -\cos 2\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

α = angle at which the plane of reflection is inclined to xz-plane

$\therefore \alpha = 0$

$2\alpha = 0$

σ_2 or $\sigma''_v(xz)$ (at 120° xz-plane).

$\alpha = 120°$

$\therefore 2\alpha = 240°$

$$= \begin{pmatrix} -1/2 & +\sqrt{3}/2 & 0 \\ +\sqrt{3}/2 & +1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\sigma_3 \text{ or } \sigma''' = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & +1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\alpha = 240°$

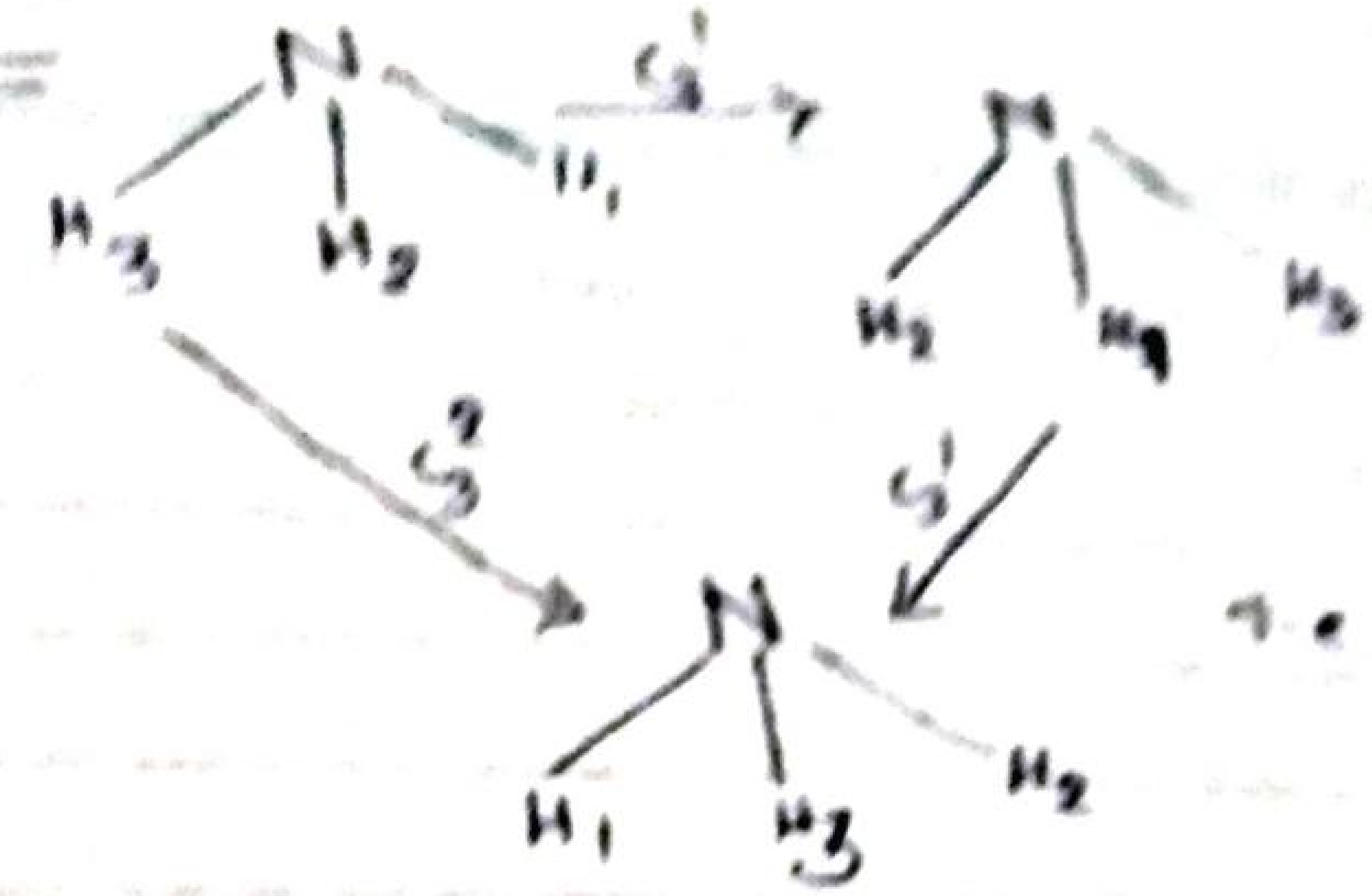
$2\alpha = 480°$ or $120°$

Multiplication table for C_{3v} group

First operation

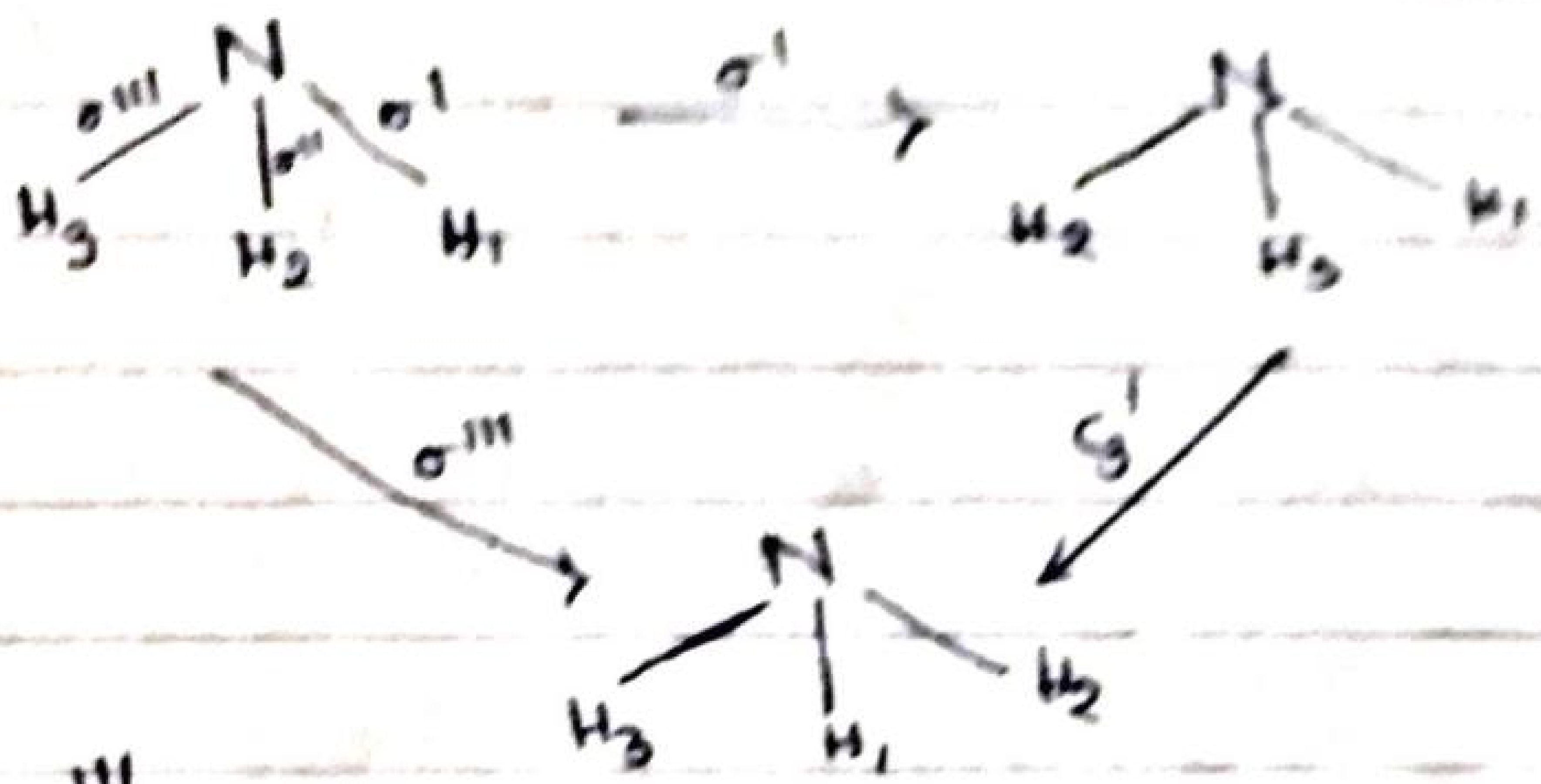
Second operation	E	C_3^1	C_3^2	σ'	σ''	σ'''
E	E	C_3^1	C_3^2	σ'	σ''	σ'''
C_3^1	C_3^1	C_3^2	E	σ'''	σ'	σ''
C_3^2	C_3^2	E	C_3^1	σ''	σ'''	σ'
σ'	σ'	σ''	σ'''	E	C_3^1	C_3^2
σ''	σ''	σ'''	σ'	C_3^2	E	C_3^1
σ'''	σ'''	σ'	σ''	C_3^1	C_3^2	E

$C_3' \cdot C_3'^{*} =$



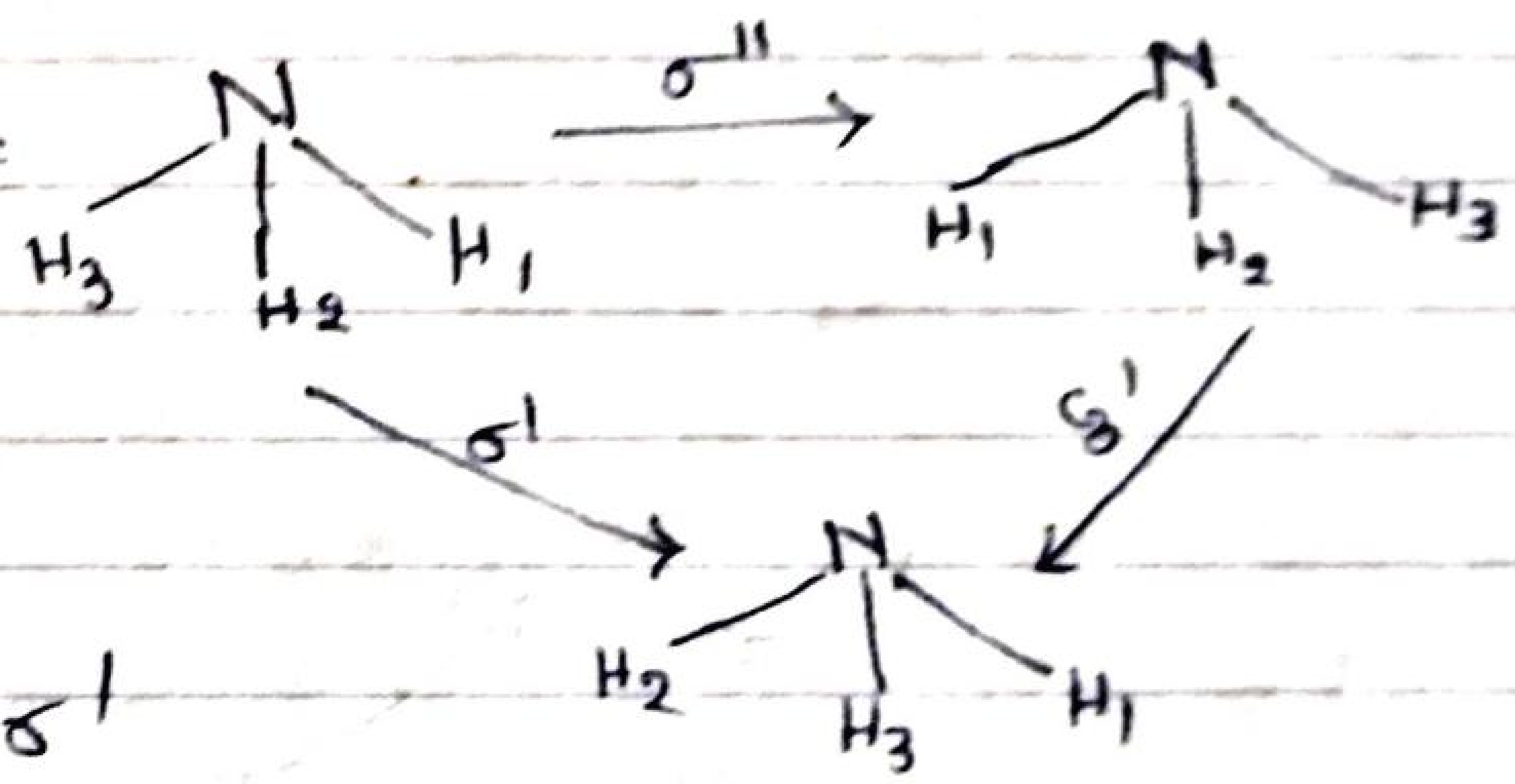
i.e. $C_3' \cdot C_3' = C_3^2$

$C_3' \cdot \sigma' =$



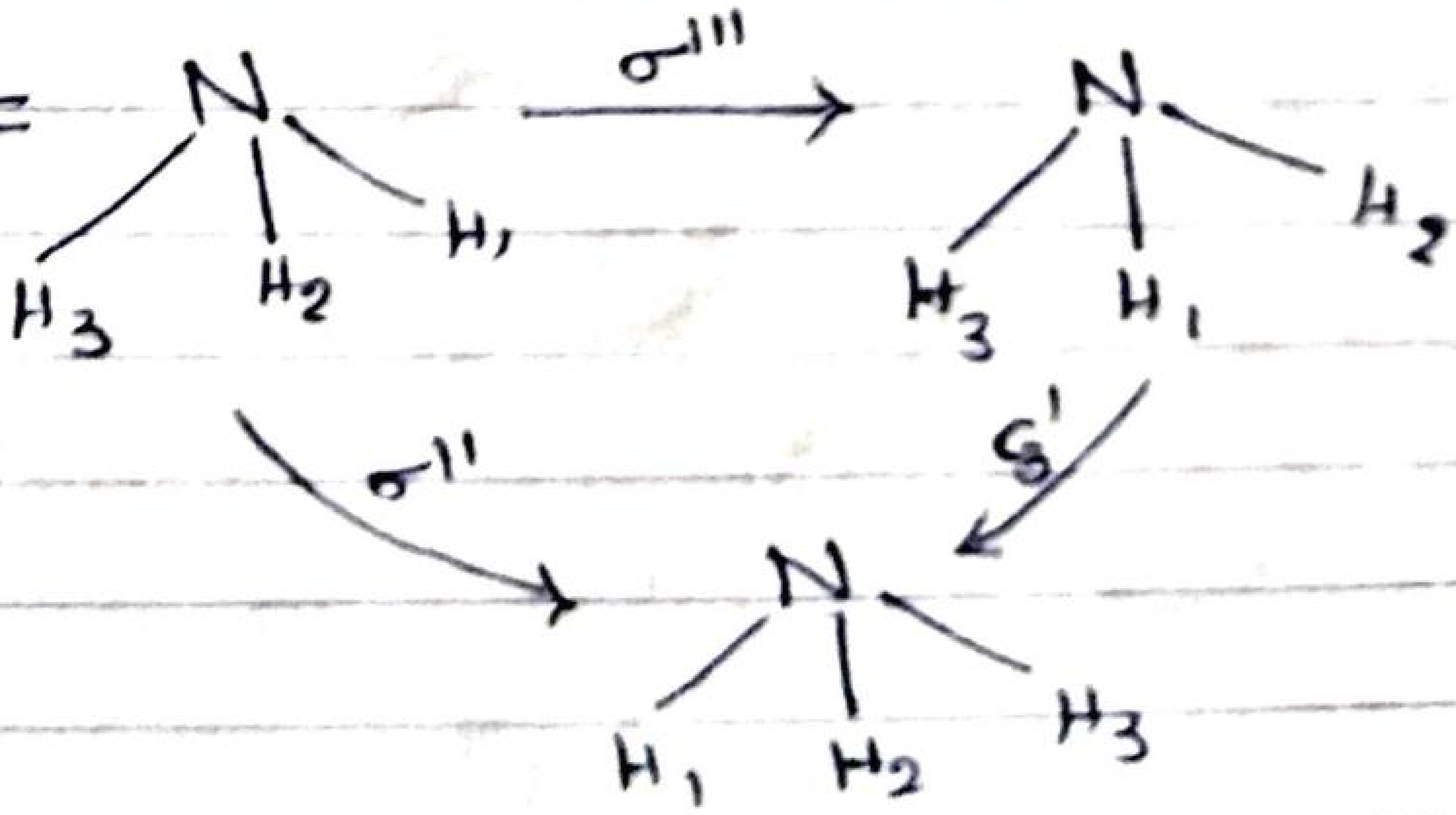
$\therefore C_3' \cdot \sigma' = \sigma'''$

$C_3' \cdot \sigma'' =$



$\therefore C_3' \cdot \sigma'' = \sigma'$

$C_3' \cdot \sigma''' =$



$\therefore C_3' \cdot \sigma''' = \sigma''$

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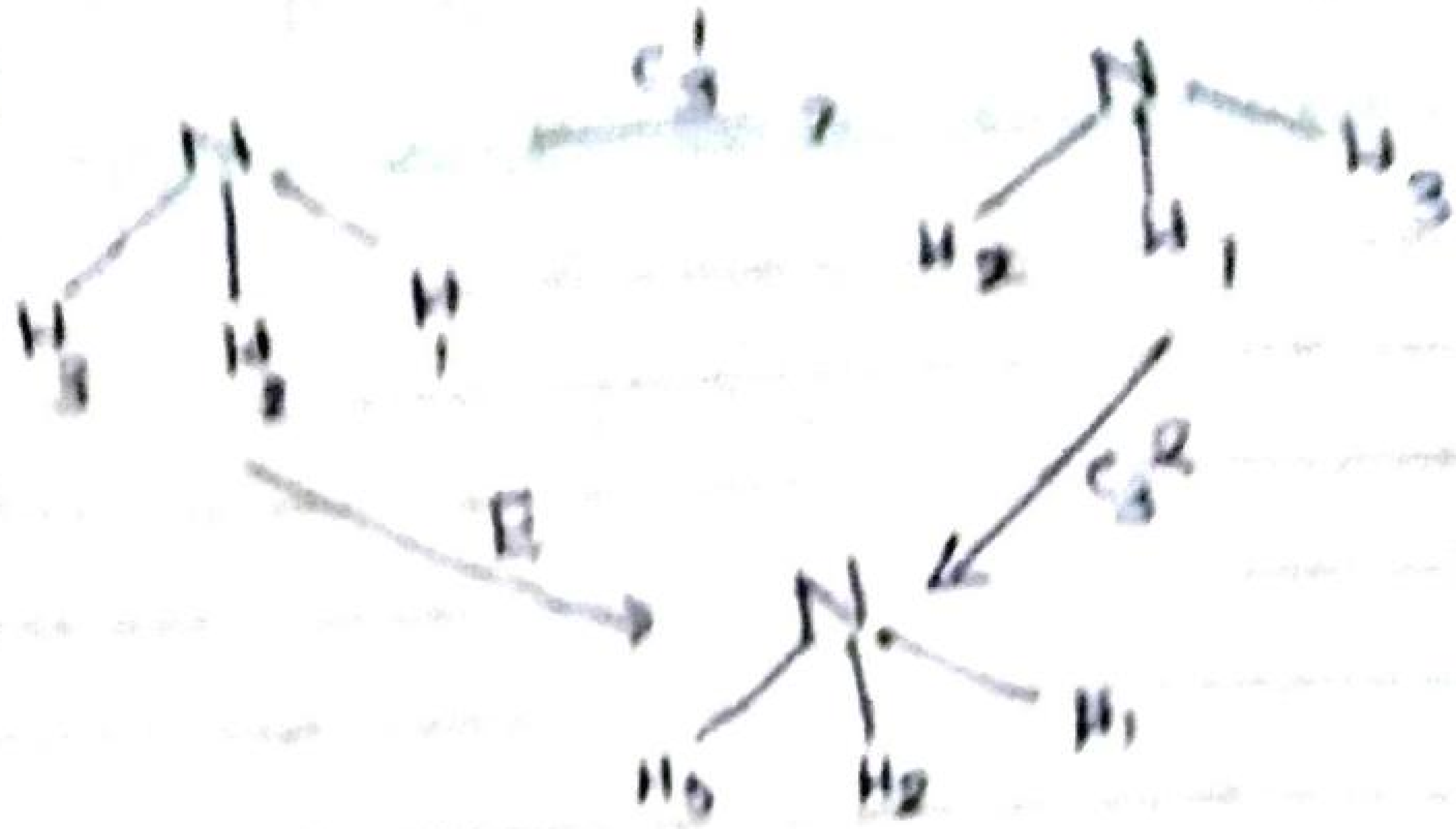
$C_3^2 \cdot C_3^1 = E$

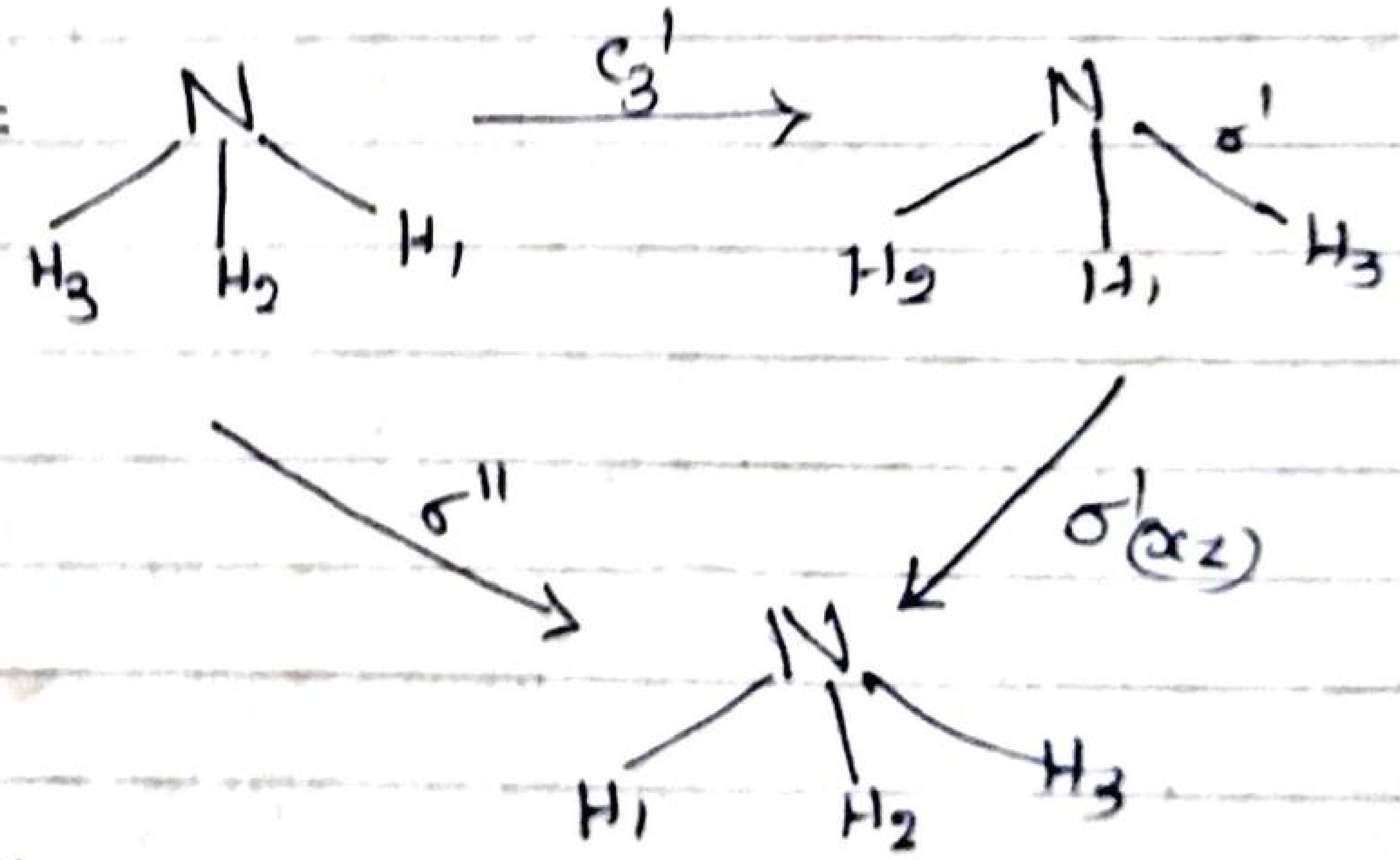


or,

$$C_3^2 \cdot C_3^1 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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

$\sigma^1 \cdot C_3^1 =$



or,

$$\sigma^1 \cdot C_3^1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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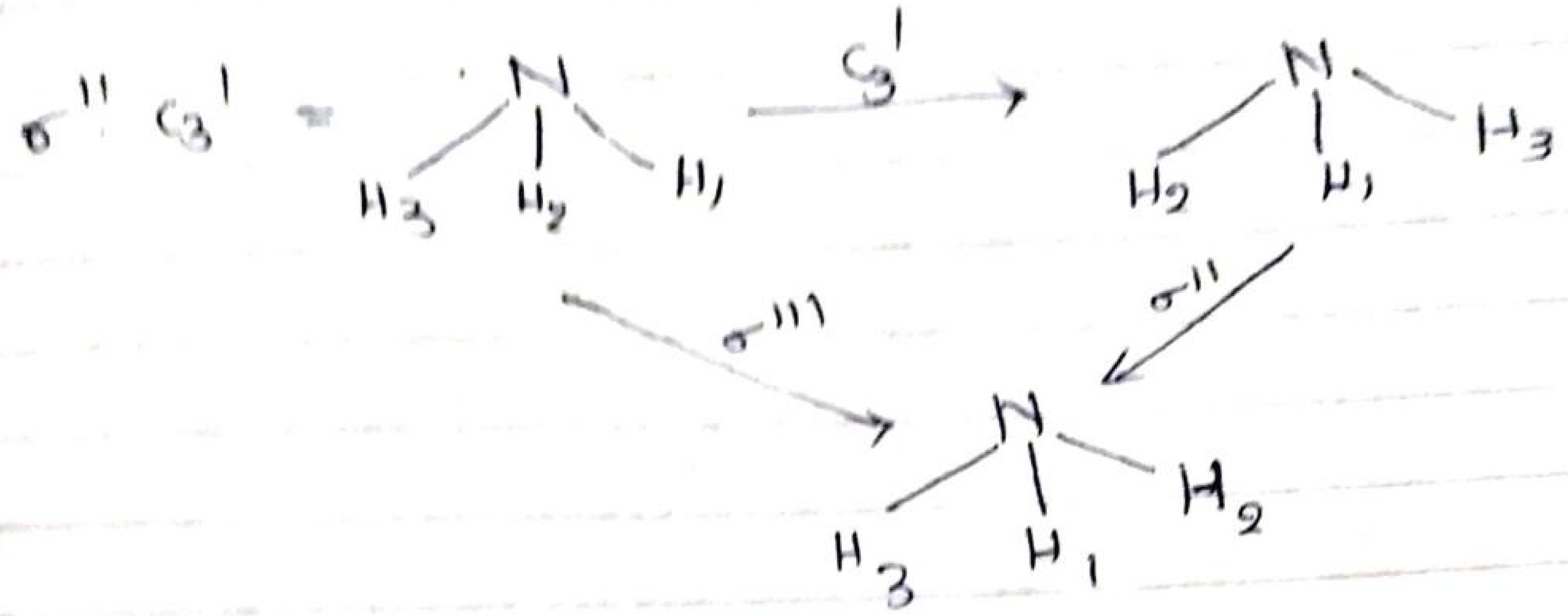
$$= \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \sigma''$$

$\sigma'' C_3' =$

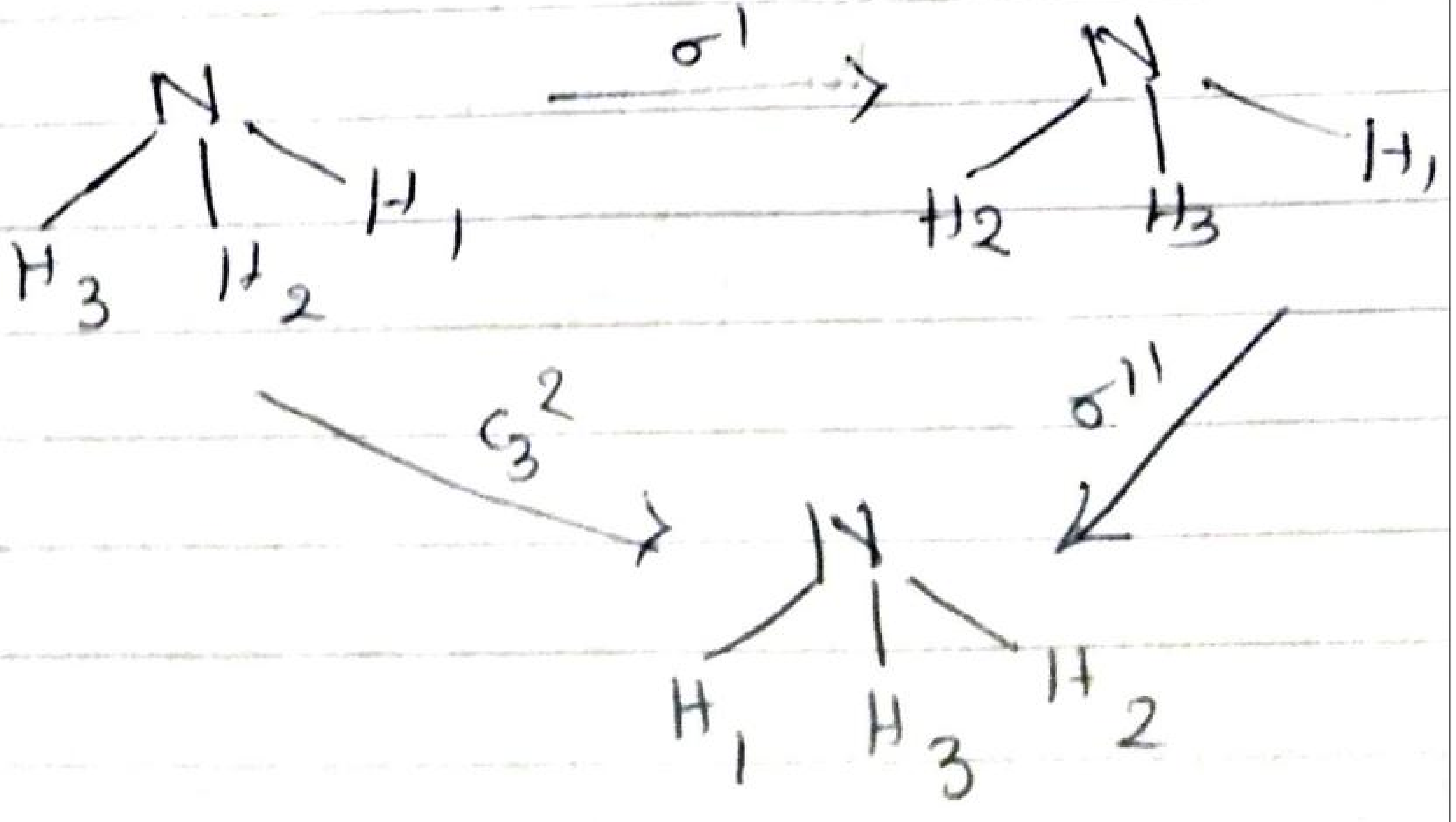


or,

$$\sigma'' \cdot C_3' = \begin{pmatrix} -1/2 & +\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & +1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & +1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \sigma'''$$

$\sigma'' \cdot \sigma' = C_3^2$



or,

$$\sigma'' \cdot \sigma' = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = C_3^2$$

Symmetry classification of molecules:

Sequence of steps :→

	Molecule type		Group
1.	Linear	Special group	$C_{\infty v}$, $D_{\infty h}$
	4 C_3 axis		T, T_h, T_d, O, O_h
	$10C_3 + 6C_5$		I, I_h

2	operation ~~only~~	group
	only a plane	C_s
	only i (centre of inversion)	C_i
	only E	C_1

3. operation — 'group'

even order only improper axis (S_4, S_6, S_8 ------) and no symm. plane or, no proper axis — S_4, S_6, S_8 --- S_n, n = even.

S_n (n = even) + any additional operation — D_n, D_{nd}, D_{nh}, --- --

4. 'operation' — 'group'

'operation'	'group'
C_n	C_n
$C_n + n\sigma_v$	C_{nv}
i.e. $C_2 + 2\sigma_v$	C_{2v}

example - 

$C_n + 1\sigma_h$	C_{nh}.

example - (trans-planar H_2O_2).

5. 'operation' — 'group'

'operation'	'group'
$C_n + nC_2$ in plane $\perp^r$ C_n	D_n, D_{nh}, D_{nd}.
$C_n + nC_2$	D_n
$C_n + nC_2$, σ_h	D_{nh}
C_n, nC_2, σ_h, $n\sigma_v$	D_{nh}.
C_n, nC_2, $n\sigma_v$	D_{nd}.