Assignment ① Matrix Representation of ops

→ To show a molecule's point group we should add vector on it & observe the effect of various symmetry operations on it.

→ By increasing no. of atoms in molecule, the number of vector increase and it become hard to observe effect of various Symm. operations.

→ So we use matrix representation

Matrix is a rectangular array of numbers or symbol for numbers (As)

$$\text{column} \downarrow \quad \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}_{3\times3} \rightarrow \text{Row}$$

→ इसमे सभी elements को column & Row मे 3-सभी position के acc. denote करते है

Matrix representation takes place in 2 parts ① column ② Row

→ as in above (pic) → a_{11} → Ist column & Ist row का element है

→ a_{21} → column No ① & row To II का element है

→ उपर (3X3) → Matrix का order है, इसको dimensions भी बोल सकते है ie 3 row & 3 column

→ order or dimension of Matrix = No. of row X No of column

→ Square Matrix → जिसमे columns & row equal (=) होते है | row = 3

→ Unit Matrix → यदि विकर्ण or diagonal पर present ele: की Value (1) हो & others की value zero है

Summation of two Matrix →

A1 → माना यह H के molecule की Matrix representation

A2 → यह इसका B

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 2 & 3 \\ 1 & 3 & 2 \end{bmatrix} + \begin{bmatrix} 2 & 0 & 3 \\ 4 & 1 & 1 \\ 5 & 0 & 3 \end{bmatrix} = \begin{bmatrix} (1+2) & (2+0) & (3+3) \\ (4+4) & (2+1) & (3+2 \\ (1+3) & (3+0) & (2+3 \end{bmatrix}$$

Substraction of two Matrix → (Ist − II)

A1 A2 B

$$\begin{bmatrix} 2 & 3 & 4 \\ 5 & 6 & 7 \\ 8 & 9 & 1 \end{bmatrix} - \begin{bmatrix} 5 & 3 & 2 \\ 0 & 3 & 0 \\ 9 & 0 & 0 \end{bmatrix} = \begin{bmatrix} -3 & 0 & 2 \\ 5 & 3 & 7 \\ -1 & 9 & 1 \end{bmatrix}$$

Multiplication of two Matrix

↳ Sts only apply in Square Matrix

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \times \begin{vmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{vmatrix}$$

↓

$$\begin{vmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{12}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{vmatrix}$$

$$\begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{12}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{bmatrix}$$

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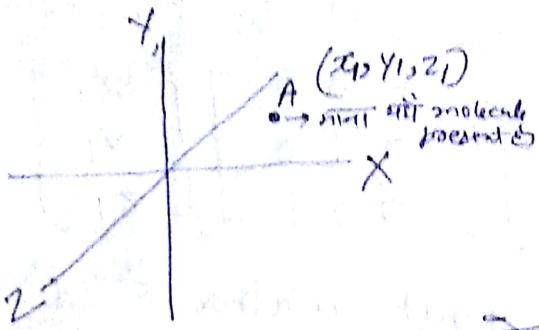
Matrix Representation for Identity :-

Identity → या तो molecular कोई symmetry operation (E) लागू नहीं करे या इसका ऐसा operation लागू किया जाये कि configuration change नहीं हो माना एक molecule (A) है जो 3 dimension में present है (Imagine) → माना molecule (A) जिसके 3 निर्देशांक x_1, y_1 & z_1 है जब इस पर operation apply करते हैं तो इसके निर्देशांक change हो जायेंगे & इन्हें ऐसे बदलेंगे कि configuration change न हो)



after apply operation

x_2, y_2, z_2 निर्देशांक हो जायेंगे

नये निर्देशांक के लिए

↳ अब इसके equation इस प्रकार से बनेंगी → निर्देशांक only उसी axis का change का होगा जिस पर operation apply करते हैं

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

↳ since इसके operation only x axis पर apply है तो वही change होगा, so इसे (1 x_1) लिखते हैं, y & z में कोई change नहीं होगा ie इसके operation के बाद only x_1 के निर्देशांक change होंगे।

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(ii) y axis में change होने पर यह होगा

$$Y_2 = 0x_1 + 1y_1 + 0z_1$$
$$Z_2 = 0x_1 + 0y_1 + 1z_1$$

इन सब तीनों का matrix represent ये होगा। →

$$\begin{bmatrix} X_1 \\ Y_2 \\ Z_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix}$$

ये Unit matrix है जिसे हम apply करते है [formula of matrix represent for identity]

It means है कि (1 0 0) x_1 के लिए, (0 1 0) y_1 के लिए & (0 0 1) z_1 के लिए है

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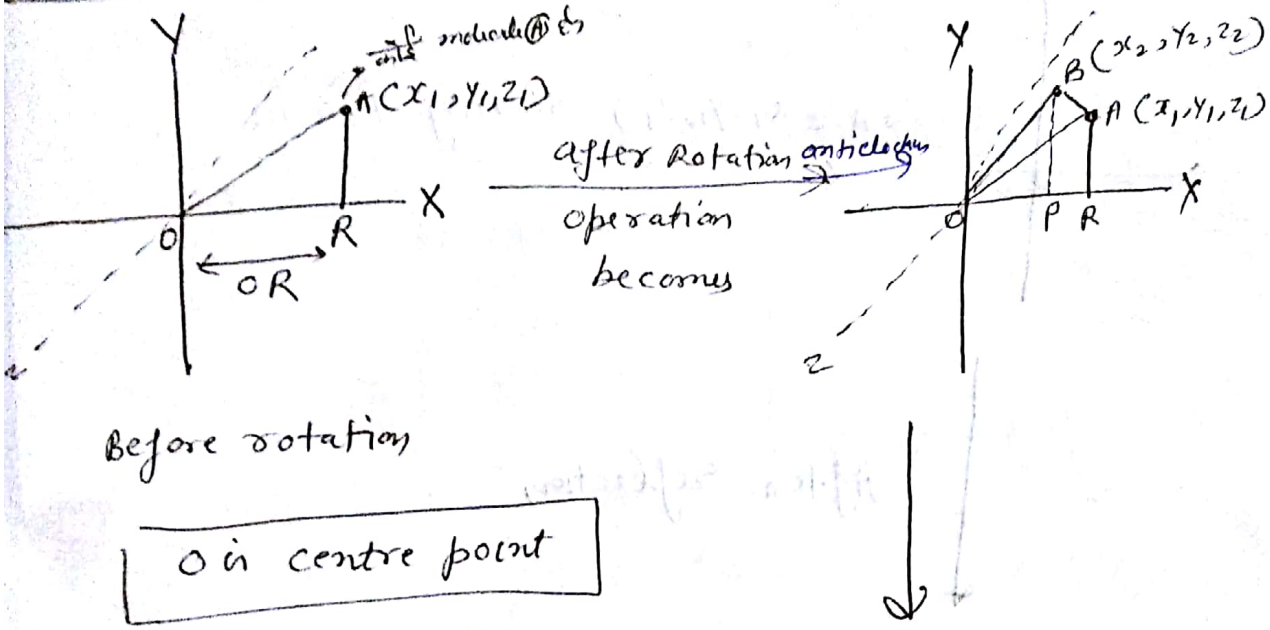
(5)

⇒ Matrix Representation for Rotation Symmetry operation (C_n)



Before rotation

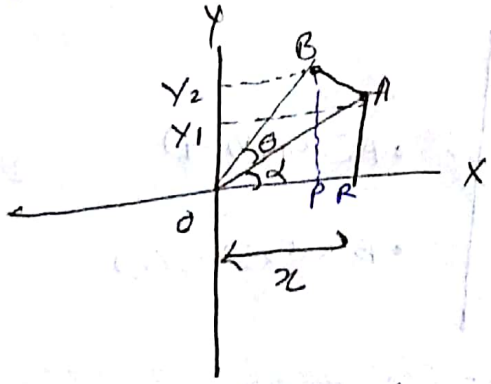
O is centre point

$OR = x_1$ → पहले का निर्देशांक

$OP = x_2$ → बाद " "

OR में cos लेते हैं sinθ

OR is bay



O

Overall Matrix representation for X, Y & Z

$$x_2 = x_1 \cos\theta - y_1 \sin\theta + 0z_1 \quad -①$$

$$y_2 = x_1 \sin\theta + y_1 \cos\theta + 0z_1 \quad -②$$

$$z_2 = 0x_1 + 0y_1 + 1z_1 \quad -③$$

since z में कोई change नहीं होते हैं so equation ③ (Identity वाली ही रहेगी)

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix}$$

↳ यहाँ rotation anticlockwise है

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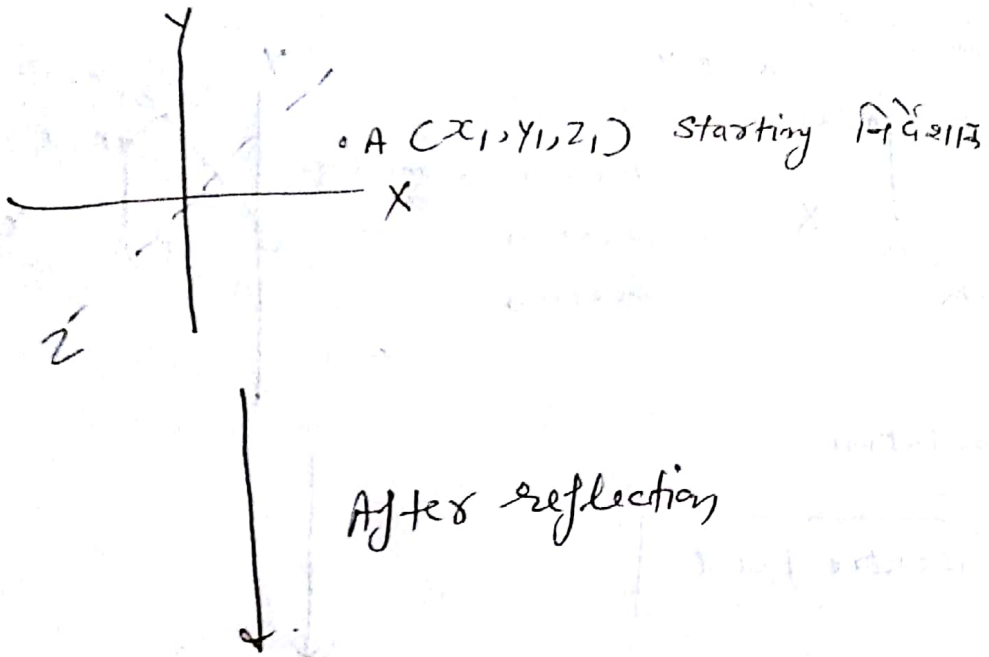
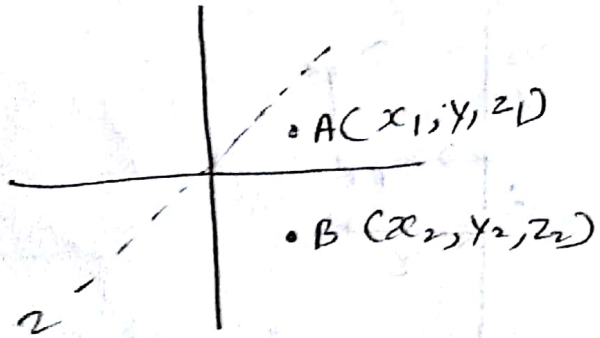
(4) Matrix representation for reflection symmetry operation





$x_2 = 1x_1 + 0y_1 + 0z_1$ निर्देशांक ⊕

$y_2 = 0x_1 + y_1 + 0z_1$ y के निर्देशांक -y

$z_2 = 0x_1 + 0y_1 + 1z_1$ ⊕ value

Matrix representation →

(x2)

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

जब reflection x2 plane से करवाया गया है

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yz plane → yz को छोड़कर x की value (-ve) होगा

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

xy plane

z (-ve)

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

(*) Matrix Representation for inversion → centre of symmetry

symmetry element C_i

$\sigma_h = xy$

$$\sigma_h = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \qquad C_i = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

यदि माना 180° से rotate कर रहे हैं

तो $\theta = 180°$

$\cos 180° = -1$

$\sin 180° = 0$

put the value C_n & S_n becomes

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

$S_n = \sigma_h \times C_n$ reflection + rotation

$$S_n = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \times \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$S_n = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$ → for improper axis of symmetry

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