PG SEMISTR II, UNIT III, SYMMETRY ELEMENTS

BY

Dr. PRIYANKA

Matrix Operations

Consider the following matrix:

Column ↓

Row →

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & a_{24} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdots & a_{3n} \\ & & & & \cdots & \\ a_{n1} & a_{n2} & a_{n2} & a_{n2} & \cdots & a_{mn} \end{bmatrix}$$

Character: **sum of diagonal elements**

In order to multiply two matrices they must be conformable, i.e., to multiply matrix A by matrix B, the number of columns in A must equal the number of rows in B.

$$(a_{11} \times b_{11}) + (a_{12} \times b_{21}) = c_{11}$$

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \end{bmatrix}$$

$$3 \times 2 \qquad 2 \times 4 \qquad = \qquad 3 \times 4$$

Row Column

The symmetry operations can all be represented mathematically as 3 × 3 square matrices.

To carry out the symmetry operation, you multiply the symmetry operation matrix times the coordinates you want to transform. The *x*, *y*, *z* coordinates are written in vector format as a 3 × 1 matrix:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

For example, the inversion operation take the general coordinates x, y, z to $-x, -y, -z$. In matrix terms we would write:

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ -z \end{bmatrix}$$

$$x(\text{new}) = (-1)(x) + (0)(y) + (0)(z)$$

$$y(\text{new}) = (0)(x) + (-1)(y) + (0)(z)$$

$$z(\text{new}) = (0)(x) + (0)(y) + (-1)(z)$$

Symmetry Operation Matrices:

E

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

i

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ -z \end{bmatrix}$$

σ(xy)

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ -z \end{bmatrix}$$

σ(xz)

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ z \end{bmatrix}$$

σ(yz)

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ y \\ z \end{bmatrix}$$

$$\mathbf{C}_{\boldsymbol{n}} \qquad \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z \end{bmatrix}$$

$$\mathbf{S}_{\boldsymbol{n}} \qquad \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ -z \end{bmatrix}$$

$$\mathbf{C}_{\boldsymbol{n}} \times \sigma_{\boldsymbol{h}} = \mathbf{S}_{\boldsymbol{n}}$$

$$\underset{\mathbf{C}_{\boldsymbol{n}}}{\begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}} \underset{\sigma_{\boldsymbol{h}}}{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}}$$