

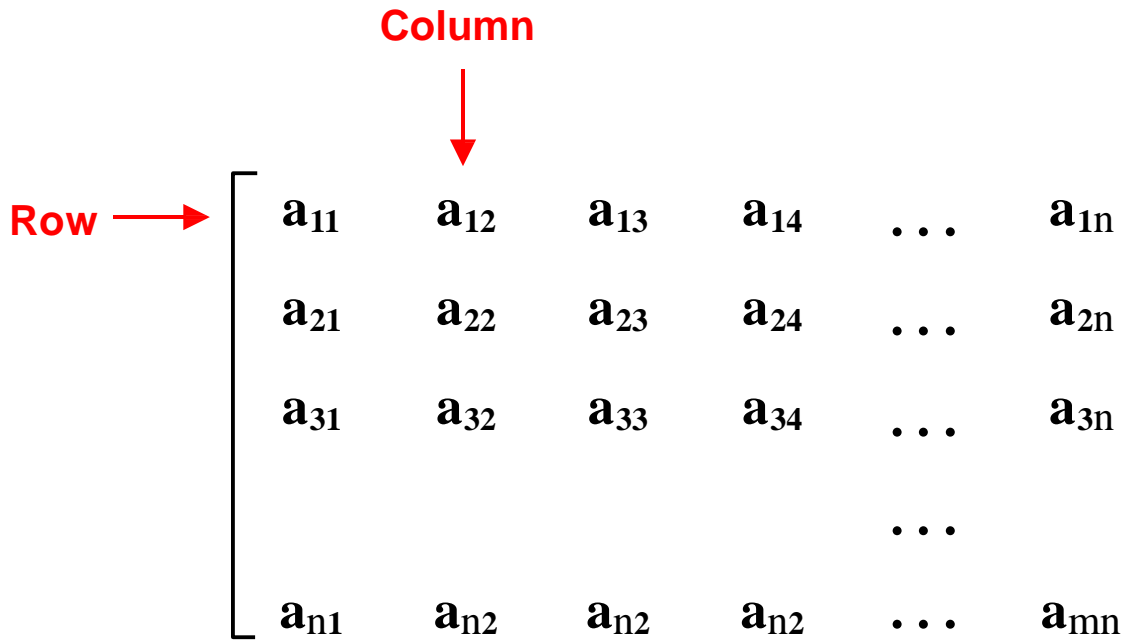
PG SEMISTR II,  
UNIT III,  
SYMMETRY  
ELEMENTS

BY

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# Matrix Operations

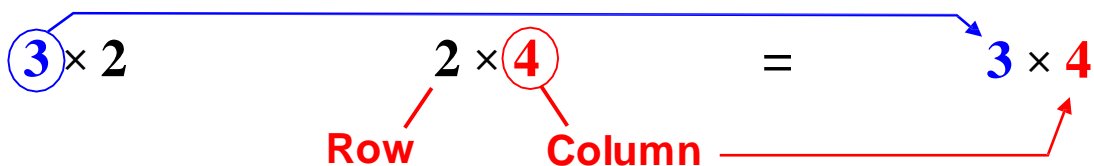
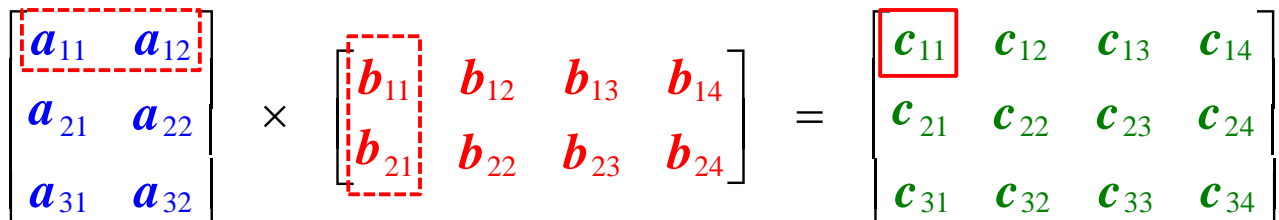
Consider the following matrix:



**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**.

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



The symmetry operations can all be represented mathematically as  $3 \times 3$  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  $3 \times 1$  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:

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

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

$$\sigma(\mathbf{xy}) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ -z \end{bmatrix}$$

$$\sigma(\mathbf{xz}) \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ z \end{bmatrix}$$

$$\sigma(\mathbf{yz}) \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ y \\ z \end{bmatrix}$$

$$C_n \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z \end{bmatrix}$$

$$S_n \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ -z \end{bmatrix}$$

$$C_n \times \sigma_h = S_n$$

$$\begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

 $C_n$ 
 $\sigma_h$