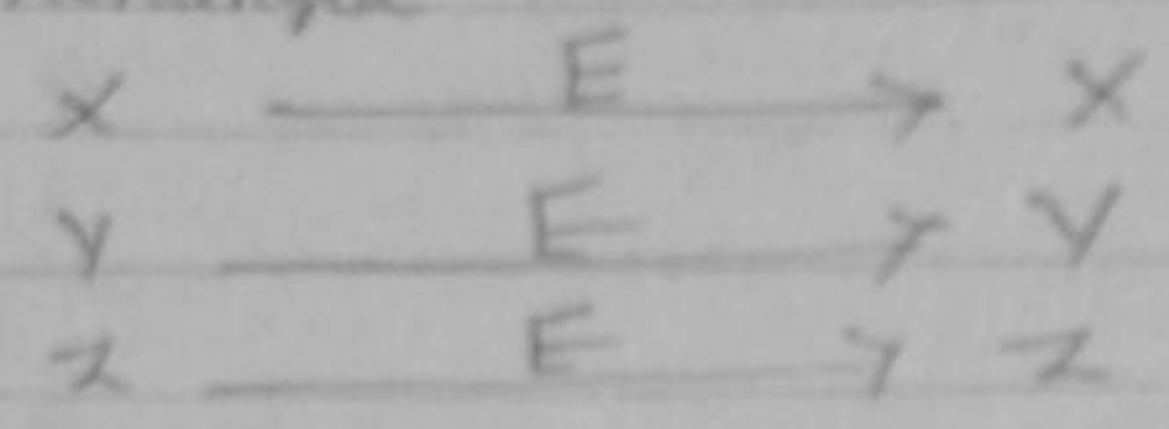


Point Groups and Character Table

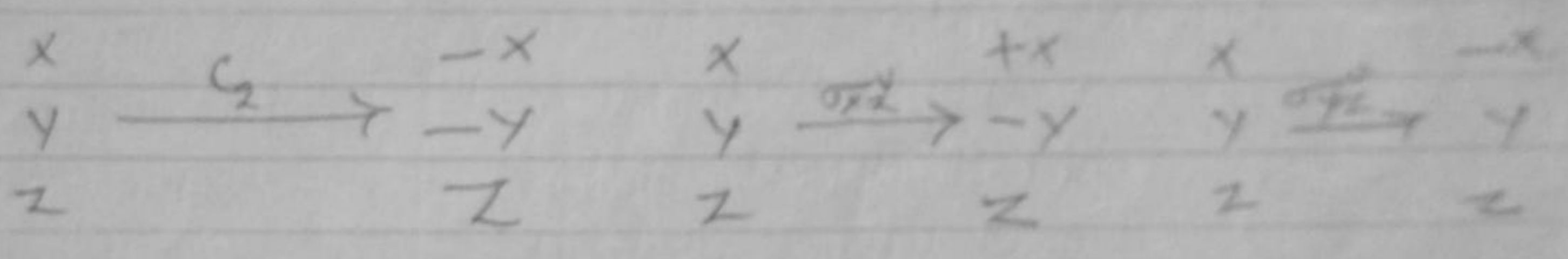
Symmetry operation and matrices: In which we will see how the symmetry operations change the co-ordinates of a molecule and what is the effect of combining two or more symmetry operations.

Let us consider the effect of the operation on the co-ordinates of a CO_2 molecule.

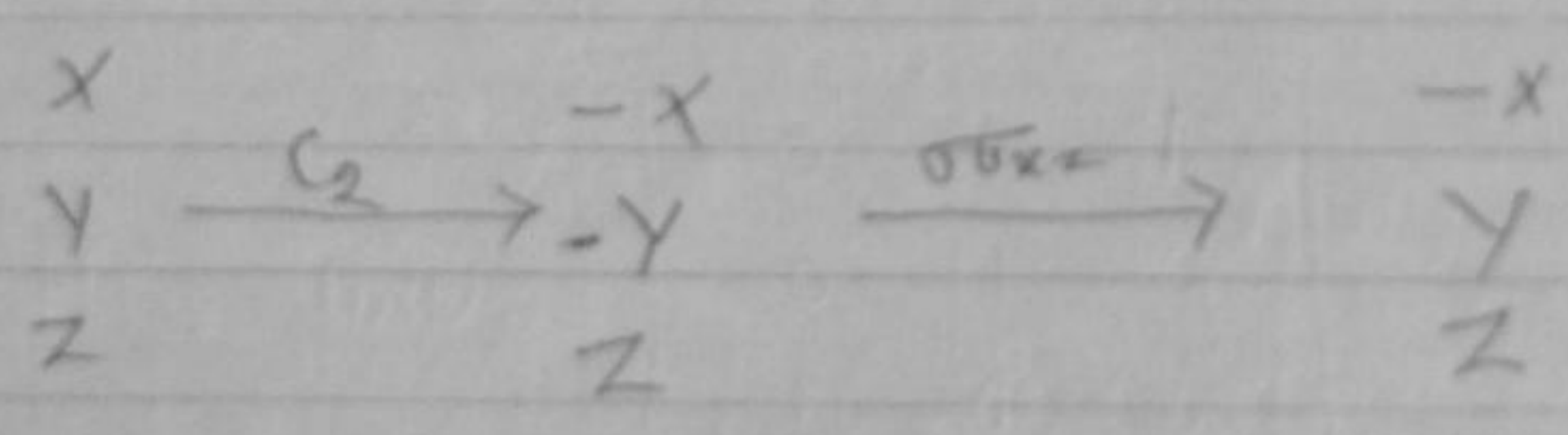
On performing E operation x, y and z remain unchanged.



On performing C_2 , σ_{xz} and σ_{yz} operation following effects will arise -



Combination of two operations can be shown as following -

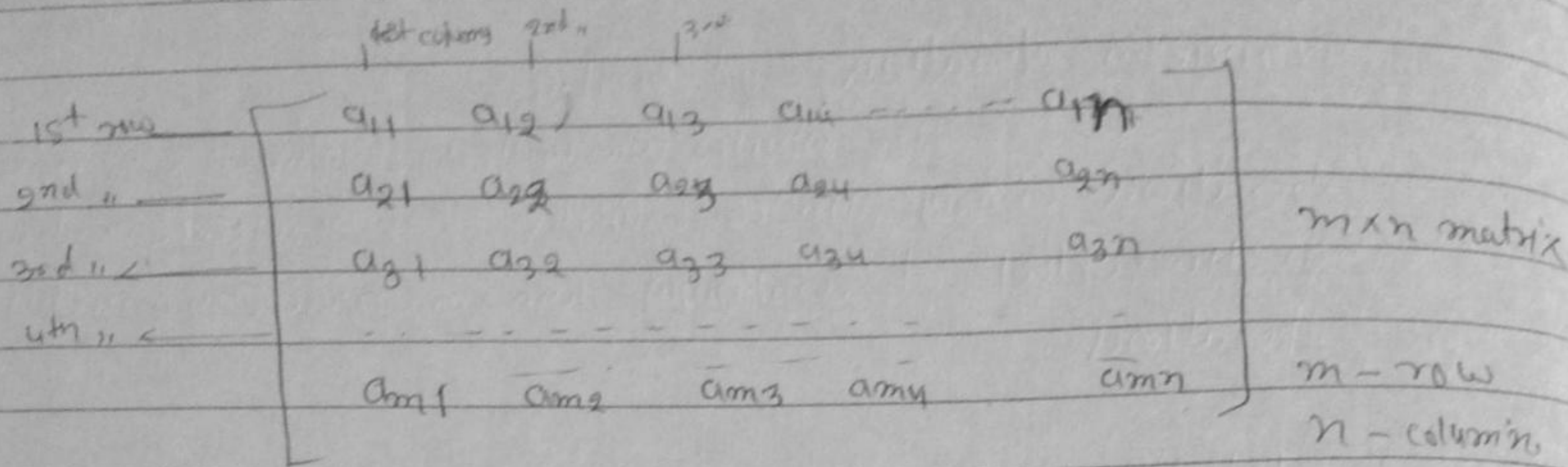


Another way of representing the operation is in the form of matrices.

Matrix \rightarrow Matrix is combination of numbers, arranged in a rectangular array, and combined with another matrix with the certain general rule. A general

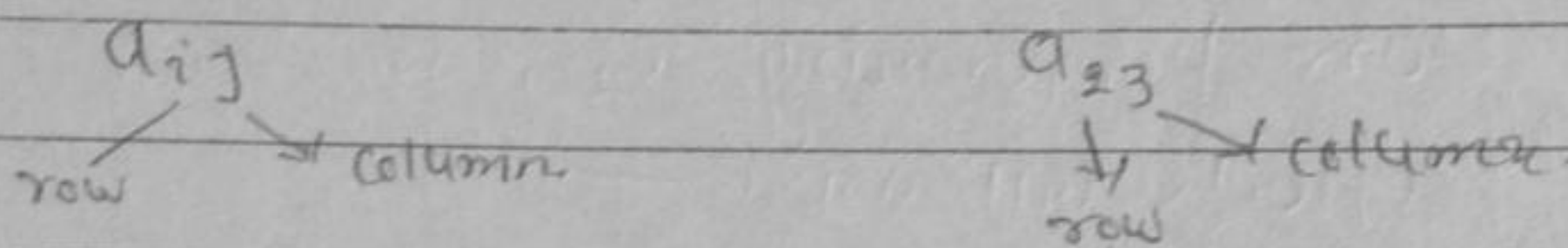
representation of the matrix will be as follows:

with n number of columns and m number of rows.



Square Matrix \rightarrow If the number of row (m) is equal to the number of column (n), a matrix is called Square matrix.

Representation of elements in the matrix \rightarrow
An element a_{ij} , represents belongs to i th row and j th column.



Diagonal matrix \rightarrow The elements which have $i = j$ are situated on the diagonal of the matrix and are called diagonal elements. For example a_{11}, a_{22}, a_{33} are diagonal elements.

Unit matrix \rightarrow The matrices in which all diagonal elements are 1 and other elements are zero, are called, unit matrices. For example

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad 3 \times 3 \quad \text{Unit matrix}$$

Sometimes Some matrix have only one ^{column} row and only one ^{row} column. These are called only single column or single row matrices. The vectors are normally represented as single column matrices and single column matrices are called vector matrices.

$$[C_2] \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix} \quad \text{hence } C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Similarly -

$$\sigma_{uxz} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ z \end{bmatrix} \quad \text{hence } \sigma_{uxz} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and } \sigma_{uyz} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

Character \rightarrow The summation of the diagonal elements of matrix is called its character. Thus character of the matrices of the different operations in C_{2v} point symmetry are.

E	C_2	σ_{uxz}	σ_{uyz}	operations
3	-1	1	1	Character

Combination of two operations can be shown as the combination of their matrices \rightarrow

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

i.e. σ_{uyz} .

Combination of different matrices can be shown in the form of a table \rightarrow

Table

	E	C_2	σ_{uxz}	σ_{uyz}
E	E	C_2	σ_{uxz}	σ_{uyz}
C_2	C_2	E	σ_{uyz}	σ_{uxz}
σ_{uxz}	σ_{uxz}	σ_{uyz}	E	C_2
σ_{uyz}	σ_{uyz}	σ_{uxz}	C_2	E

The symm operations can be considered as elements. The molecule can be considered to be a set of elements