Matrices and Symmetry

The algebra of matrices is ideal for describing the symmetry elements of molecules.

Matrices can be used with varying degrees of sophistication – the simplest is to use them to operate on atomic labels.

A Simple Example

The configuration of this triangular molecule can be represented by a column matrix

\[
\begin{pmatrix} A \\ B \\ C \end{pmatrix}
\]

Any symmetry operation can be characterised by its effect on the column matrix – and thus can be represented as a (3x3) matrix

Rotation Clockwise by 120°

Reflections / Mirror Planes

Combining Operations – R then \( \sigma \)

Combining Operations - \( \sigma \) then R

Apply \( R_{120} \) then \( \sigma \)

Apply \( \sigma \) then \( R_{120} \)
Summary

The column vector conveniently represents the essentials of the molecular topology.

Symmetry operations can be represented by matrices.

The normal rules of matrix multiplication reproduce application of multiple symmops.

A non-commutative algebra.

General Rotations

- In the normal X,Y system P is (x,y).
- In the rotated X′, Y′ system P is (x′,y′)

\[ x' = x \cos(\alpha) + y \sin(\alpha) \]
\[ y' = -x \sin(\alpha) + y \cos(\alpha) \]

Rotation Matrices – 2D

Rewriting as a matrix equation

\[
\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = R_\alpha \begin{pmatrix} x \\ y \end{pmatrix}
\]

The operation “rotate the coordinate system anti-clockwise by \( \alpha \)”, is identical to “rotate objects clockwise by \( \alpha \)”

The operation is implemented by multiplying the matrix onto the coordinates of any object.

Rotation Matrices – 3D

Rotation about the z-axis

\[
\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) & 0 \\ -\sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = R_z(\alpha) \begin{pmatrix} x \\ y \\ z \end{pmatrix}
\]

Or the x axis...

\[
\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha) & \sin(\alpha) \\ 0 & -\sin(\alpha) & \cos(\alpha) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = R_x(\alpha) \begin{pmatrix} x \\ y \\ z \end{pmatrix}
\]