Matrix representation of symmetry operations

Using carthesian coordinates (x,y,z) or some **position vector**, we are able to define an initial position of a point or an atom.

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

The initial vector is submitted to a symmetry operation and thereby transformed into some resulting vector defined by the coordinates x', y' and z'. In an algebraic context, this transformation is expressed a matrix which processes the initial position vector. We write

*final vector = Matrix * initial vector.*

The most primitive symmetry operation is the identity and yields a final vector identical to the initial vector. It is the **unity matrix** or **identity matrix** which leaves all coordiates unaffected.

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

If we want to perform a **reflection** on the xy-plane (analogous to a horizontal plane σ_h), coordinate z changes the sign.

$$\sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

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

The matrices which are applied for performing a reflection on the yz-plane and xz-plane are the matrices σ_x and σ_y respectively.

$$\sigma_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The **inversion *i*** relates the coordinates (x,y,z) with (-x,-y,-z) and is connected with the following matrix:

$$i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Obviously, a twofold application of the inversion matrix yields the coordinates of the initial point (x,y,z) which is reflected by ***E = i*i***.

$$i \cdot i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = E$$

The matrix for a rotation about axis z by an arbitrary angle Θ is derived easily if we imagine two two-dimensional coordinate planes with identical origin but an angular difference of Θ between the axes. In our context of symmetry, we just need to deal with the discrete values of $\Theta = 2\pi/n$ for the angle of rotation.

$$C_n = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The matrices for the symmetry operations $C_2(z)$, $C_3(z)$, $C_4(z)$, $C_5(z)$ and $C_6(z)$ are obtained easily. The matrices for C_n^m as symmetry operation are calculated by an n-fold multiplication of matrix C_n. The symmetry operation C_2 around axis x (x→x,y→-y, z→-z) and around axis y are (x→-x, y→y, z→-z):

$$C_2(x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad C_2(y) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

As we know rotatory-reflection to be a combination of rotation and reflection, a matrix representation for this operation is easily to be derived. For instance, to obtain the matrix for rotatory reflection $S_n(z)$ we multiply the matrices for the fundamental operations &sigma$_z$ and C_n.

$$S_n(z) = \sigma_z C_n = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & -1 \end{pmatrix}$$