PROOF

$$\chi_{\mathscr{C}} = \sum_j c_{jj} = \sum_j \sum_k a_{jk} b_{kj}$$

$$\chi_{\mathscr{D}} = \sum_k d_{kk} = \sum_k \sum_j b_{kj} a_{jk}$$

$$= \sum_j \sum_k b_{kj} a_{jk} = \sum_j \sum_k a_{jk} b_{kj} = \chi_{\mathscr{C}}$$

Conjugate matrices have identical characters.

Conjugate matrices are related by a similarity transformation in the same way as are conjugate elements of a group. Thus, if matrices $\mathscr{R}$ and $\mathscr{P}$ are conjugate, there is some other matrix $\mathscr{Q}$ such that

$$\mathscr{R} = \mathscr{Q}^{-1} \mathscr{P} \mathscr{Q}$$

Since the associative law holds for matrix multiplication, the theorem is proved in the following way.

PROOF

$$\chi \text{ of } \mathscr{R} = \chi \text{ of } \mathscr{Q}^{-1}\mathscr{P}\mathscr{Q} = \chi \text{ of } (\mathscr{Q}^{-1}\mathscr{P})\mathscr{Q}$$

$$= \chi \text{ of } \mathscr{Q}(\mathscr{Q}^{-1}\mathscr{P}) = \chi \text{ of } (\mathscr{Q}\mathscr{Q}^{-1})\mathscr{P}$$

$$= \chi \text{ of } \mathscr{P}$$

Matrix Notation for Geometric Transformations

One important application of matrix algebra is in expressing the transformations of a point—or the collection of points that define a body—in space. We have employed previously five types of operations in describing the symmetry of a molecule or other object: E, σ, i, C_n, S_n. Each of these types of operation can be described by a matrix.

The Identity. When a point with coordinates x, y, z is subjected to the identity operation, its new coordinates are the same as the initial ones, namely, x, y, z. This may be expressed in a matrix equation as

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

Thus, the identity operation is described by a unit matrix.

Reflections. If a plane of reflection is chosen to coincide with a principal Cartesian plane (i.e., an xy, xz, or yz plane), reflection of a general point has the effect of changing the sign of the coordinate measured perpendicular to the plane while leaving unchanged the two coordinates whose axes define the plane. Thus, for reflections in the three principal planes, we may write the following matrix equations:

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

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

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

Inversion. To simply change the signs of all the coordinates without permuting any, we clearly need a *negative* unit matrix, namely,

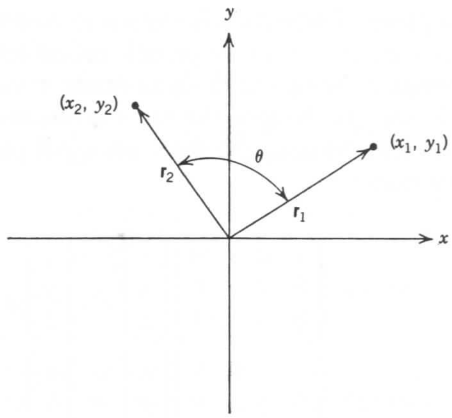
$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \bar{x} \\ \bar{y} \\ \bar{z} \end{bmatrix}$$

Proper Rotation. Defining the rotation axis as the z axis, we note first that the z coordinate will be unchanged by any rotation about the z axis. Thus, the matrix we seek must be, in part,

$$\begin{bmatrix} & & 0 \\ & & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The problem of finding the four missing elements can then be solved as a two-dimensional problem in the xy plane.

Suppose that we have a point in the xy plane with coordinates x_1 and y_1, as shown in the diagram. This point defines a vector, $\mathbf{r}_1$, between itself and the origin. Now suppose that this vector is rotated through an angle θ so that a new vector, $\mathbf{r}_2$, is produced with a terminus at the point x_2 and y_2. We now inquire about how the final coordinates, x_2 and y_2, are related to the original coordinates, x_1 and y_1, and the angle θ. The relationship is not difficult to work out. When the x component of $\mathbf{r}_1$, x_1, is rotated by θ, it becomes a vector $\mathbf{x}'$ which has an x component of $x_1 \cos\theta$ and a y component of $x_1 \sin\theta$.



Similarly, the y component of $\mathbf{r}_1$, y_1, upon rotation by θ becomes a new vector $\mathbf{y}'$, which has an x component of $-y_1 \sin\theta$ and a y component of $y_1 \cos\theta$. Now, x_2 and y_2, the components of $\mathbf{r}_2$, must be equal to the sums of the x and y components of $\mathbf{x}'$ and $\mathbf{y}'$, so we write

$$\begin{aligned} x_2 &= x_1 \cos\theta - y_1 \sin\theta \\ y_2 &= x_1 \sin\theta + y_1 \cos\theta \end{aligned} \tag{4.1-1}$$

The transformation expressed by 4.1-1 can be written in matrix notation in the following way:

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}$$

This result is for a counterclockwise rotation. Because $\cos\phi = \cos(-\phi)$ while $\sin\phi = -\sin(-\phi)$, the matrix for a clockwise rotation through the angle ϕ must be

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

Thus, finally, the total matrix equation for a clockwise rotation through ϕ about the z axis is

$$\begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix}$$

Improper Rotation. Since an improper rotation through the angle ϕ about the z axis produces the same transformation of the x and y coordinates as does a proper rotation through the same angle, but in addition changes the