THE CHEMIST'S TOOLKIT 24 Matrices

A **matrix** is an array of numbers arranged in a certain number of rows and a certain number of columns; the numbers of rows and columns may be different. The rows and columns are numbered 1, 2, … so that the number at each position in the matrix, called the **matrix element**, has a unique row and column index. The element of a matrix $\boldsymbol{M}$ at row r and column c is denoted M_{rc}. For instance, a 3×3 matrix is

$$\boldsymbol{M} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix}$$

The **trace** of a matrix, Tr $\boldsymbol{M}$, is the sum of the diagonal elements.

$$\mathrm{Tr}\,\boldsymbol{M} = \sum_n M_{nn} \qquad (24.1)$$

In this case

$$\mathrm{Tr}\,\boldsymbol{M} = M_{11} + M_{22} + M_{33}$$

A **unit** matrix has diagonal elements equal to 1 and all other elements zero. A 3×3 unit matrix is therefore

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

Matrices are added by adding the corresponding matrix elements. Thus, to add the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ to give the sum $\boldsymbol{S} = \boldsymbol{A} + \boldsymbol{B}$, each element of $\boldsymbol{S}$ is given by

$$S_{rc} = A_{rc} + B_{rc} \qquad (24.2)$$

Only matrices of the same dimensions can be added together.

Matrices are multiplied to obtain the product $\boldsymbol{P} = \boldsymbol{AB}$; each element of $\boldsymbol{P}$ is given by

$$P_{rc} = \sum_n A_{rn} B_{nc} \qquad (24.3)$$

Matrices can be multiplied only if the number of columns in $\boldsymbol{A}$ is equal to the number of rows in $\boldsymbol{B}$. Square matrices (those with the same number of rows and columns) can therefore be multiplied only if both matrices have the same dimension (that is, both are $n \times n$). The products $\boldsymbol{AB}$ and $\boldsymbol{BA}$ are not necessarily the same, so matrix multiplication is in general 'non-commutative'.

Brief illustration 24.1: Matrix addition and multiplication

Consider the matrices

$$\boldsymbol{M} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \text{ and } \boldsymbol{N} = \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix}$$

Their sum is

$$\boldsymbol{S} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} + \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix} = \begin{pmatrix} 6 & 8 \\ 10 & 12 \end{pmatrix}$$

and their product is

$$\boldsymbol{P} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix} = \begin{pmatrix} 1\times5+2\times7 & 1\times6+2\times8 \\ 3\times5+4\times7 & 3\times6+4\times8 \end{pmatrix}$$

$$= \begin{pmatrix} 19 & 22 \\ 43 & 50 \end{pmatrix}$$

An $n \times 1$ matrix (with n elements in one column) is called a **column vector**. It may be multiplied by a square $n \times n$ matrix to generate a new column vector, as in

$$\begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \times \begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix}$$

The elements of the two column vectors need only one index to indicate their row. Each element of $\boldsymbol{P}$ is given by

$$P_r = \sum_n A_{rn} B_n \qquad (24.4)$$

A $1 \times n$ matrix (a single row with n elements) is called a **row vector**. It may be multiplied by a square $n \times n$ matrix to generate a new row vector, as in

$$(P_1\ P_2\ P_3) = (B_1\ B_2\ B_3) \times \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}$$

In general the elements of $\boldsymbol{P}$ are

$$P_c = \sum_n B_n A_{nc} \qquad (24.5)$$

Note that a column vector is multiplied 'from the left' by the square matrix and a row vector is multiplied 'from the right'. The **inverse** of a matrix $\boldsymbol{A}$, denoted $\boldsymbol{A}^{-1}$, has the property that $\boldsymbol{AA}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \mathbf{1}$, where $\mathbf{1}$ is a unit matrix with the same dimensions as $\boldsymbol{A}$.

Brief illustration 24.2: Inversion

Mathematical software gives the following inversion of a matrix $\boldsymbol{A}$:

Matrix	Inverse
$\boldsymbol{A}$	$\boldsymbol{A}^{-1}$
$\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$	$\boldsymbol{A}^{-1} = \begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix}$