THE CHEMIST'S TOOLKIT 4 Integration

Integration is concerned with the areas under curves. The **integral** of a function $f(x)$, which is denoted $\int f(x)\mathrm{d}x$ (the symbol $\int$ is an elongated S denoting a sum), between the two values $x = a$ and $x = b$ is defined by imagining the x-axis as divided into strips of width δx and evaluating the following sum:

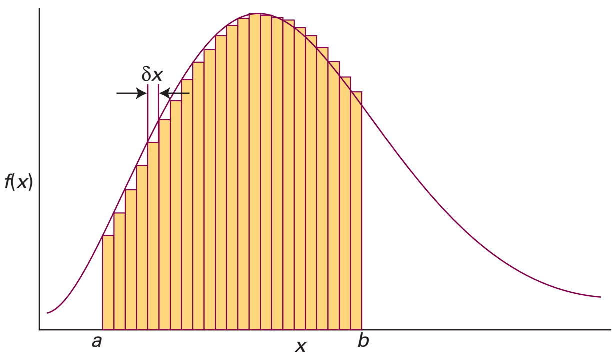
$$\int_a^b f(x)\mathrm{d}x = \lim_{\delta x \to 0} \sum_i f(x_i)\delta x \qquad \text{Integration [definition]} \qquad (4.1)$$

As can be appreciated from Sketch 4.1, the integral is the area under the curve between the limits a and b. The function to be integrated is called the **integrand**. It is an astonishing mathematical fact that the integral of a function is the inverse of the differential of that function. In other words, if differentiation of f is followed by integration of the resulting function, the result is the original function f (to within a constant).

The integral in the preceding equation with the limits specified is called a **definite integral**. If it is written without the limits specified, it is called an **indefinite integral**. If the result of carrying out an indefinite integration is $g(x) + C$, where C is a constant, the following procedure is used to evaluate the corresponding definite integral:

$$I = \int_a^b f(x)\mathrm{d}x = \{g(x)+C\}\Big|_a^b = \{g(b)+C\} - \{g(a)+C\}$$
$$= g(b) - g(a) \qquad \text{Definite integral} \qquad (4.2)$$

Note that the constant of integration disappears. The definite and indefinite integrals encountered in this text are listed in the *Resource section*. They may also be calculated by using mathematical software.



Sketch 4.1

Further information

When an indefinite integral is not in the form of one of those listed in the *Resource section* it is sometimes possible to transform it into one of these forms by using integration techniques such as:

Integration by parts. See *The chemist's toolkit* 15.

Substitution. Introduce a variable u related to the independent variable x (for example, an algebraic relation such as $u = x^2 - 1$ or a trigonometric relation such as $u = \sin x$). Express the differential $\mathrm{d}x$ in terms of $\mathrm{d}u$ (for these substitutions, $\mathrm{d}u = 2x\,\mathrm{d}x$ and $\mathrm{d}u = \cos x\,\mathrm{d}x$, respectively). Then transform the original integral written in terms of x into an integral in terms of u for which, in some cases, a standard form such as one of those listed in the *Resource section* can be used.

Brief illustration 4.1: Integration by substitution

To evaluate the indefinite integral $\int \cos^2 x \sin x\,\mathrm{d}x$ make the substitution $u = \cos x$. It follows that $\mathrm{d}u/\mathrm{d}x = -\sin x$, and therefore that $\sin x\,\mathrm{d}x = -\mathrm{d}u$. The integral is therefore

$$\int \cos^2 x \sin x\,\mathrm{d}x = -\int u^2\mathrm{d}u = -\tfrac{1}{3}u^3 + C = -\tfrac{1}{3}\cos^3 x + C$$

To evaluate the corresponding definite integral, convert the limits on x into limits on u. Thus, if the limits are $x = 0$ and $x = \pi$, the limits become $u = \cos 0 = 1$ and $u = \cos \pi = -1$:

$$\int_0^\pi \cos^2 x \sin x\,\mathrm{d}x = -\int_1^{-1} u^2\mathrm{d}u = \left\{-\tfrac{1}{3}u^3 + C\right\}\Big|_1^{-1} = \tfrac{2}{3}$$

A function may depend on more than one variable, in which case it may be necessary to integrate over all the variables, as in:

$$I = \int_a^b \int_c^d f(x,y)\mathrm{d}x\mathrm{d}y$$

We (but not everyone) adopt the convention that a and b are the limits of the variable x and c and d are the limits for y (as depicted by the colours in this instance). This procedure is simple if the function is a product of functions of each variable and of the form $f(x,y) = X(x)Y(y)$. In this case, the double integral is just a product of each integral:

$$I = \int_a^b \int_c^d X(x)Y(y)\mathrm{d}x\mathrm{d}y = \int_a^b X(x)\mathrm{d}x \int_c^d Y(y)\mathrm{d}y$$

Brief illustration 4.2: A double integral

Double integrals of the form

$$I = \int_0^{L_1}\int_0^{L_2} \sin^2(\pi x/L_1)\sin^2(\pi y/L_2)\mathrm{d}x\mathrm{d}y$$

occur in the discussion of the translational motion of a particle in two dimensions, where L_1 and L_2 are the maximum extents of travel along the x- and y-axes, respectively. To evaluate I write

$$I = \overbrace{\int_0^{L_1} \sin^2(\pi x/L_1)\mathrm{d}x}^{\text{Integral T.2}} \overbrace{\int_0^{L_2} \sin^2(\pi y/L_2)\mathrm{d}y}^{\text{Integral T.2}}$$
$$= \left\{\tfrac{1}{2}x - \frac{\sin(2\pi x/L_1)}{4\pi/L_1} + C\right\}\Bigg|_0^{L_1} \left\{\tfrac{1}{2}y - \frac{\sin(2\pi y/L_2)}{4\pi/L_2} + C\right\}\Bigg|_0^{L_2}$$
$$= \tfrac{1}{4}L_1 L_2$$