THE CHEMIST'S TOOLKIT 15 Integration by parts

Many integrals in quantum mechanics have the form $\int f(x)h(x)\mathrm{d}x$, where $f(x)$ and $h(x)$ are two different functions. Such integrals can often be evaluated by regarding $h(x)$ as the derivative of another function, $g(x)$, such that $h(x) = \mathrm{d}g(x)/\mathrm{d}x$. For instance, if $h(x) = x$, then $g(x) = \frac{1}{2}x^2$. The integral is then found using **integration by parts**:

$$\int f\frac{\mathrm{d}g}{\mathrm{d}x}\mathrm{d}x = fg - \int g\frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x \qquad (15.1a)$$

The procedure is successful only if the integral on the right turns out to be one that can be evaluated more easily than the one on the left. The procedure is often summarized by expressing this relation as

$$\int f\mathrm{d}g = fg - \int g\mathrm{d}f \qquad (15.1b)$$

Brief illustration 15.1: Integration by parts

Integrals over xe^{-ax} and their analogues occur commonly in the discussion of atomic structure and spectra. They may be integrated by parts, as in the following. Consider integration of xe^{-ax}. In this case, $f(x) = x$, so $\mathrm{d}f(x)/\mathrm{d}x = 1$ and $\mathrm{d}g(x)/\mathrm{d}x = e^{-ax}$, so $g(x) = -(1/a)e^{-ax}$. Then

$$\int \overbrace{x}^{f}\,\overbrace{e^{-ax}}^{\mathrm{d}g/\mathrm{d}x}\,\mathrm{d}x = \overbrace{x}^{f}\,\overbrace{\frac{-e^{-ax}}{a}}^{g} - \int \overbrace{\frac{-e^{-ax}}{a}}^{g}\,\overbrace{1}^{\mathrm{d}f/\mathrm{d}x}\,\mathrm{d}x$$

$$= -\frac{xe^{-ax}}{a} + \frac{1}{a}\int e^{-ax}\mathrm{d}x = -\frac{xe^{-ax}}{a} - \frac{e^{-ax}}{a^2} + \text{constant}$$

If the integral is definite, then apply the limits to the final step above and write

$$\int_0^\infty \overbrace{x}^{f}\,\overbrace{e^{-ax}}^{\mathrm{d}g/\mathrm{d}x}\,\mathrm{d}x = \overbrace{x}^{f}\,\overbrace{\frac{-e^{-ax}}{a}}^{g}\Big|_0^\infty - \int_0^\infty \overbrace{\frac{-e^{-ax}}{a}}^{g}\,\overbrace{1}^{\mathrm{d}f/\mathrm{d}x}\,\mathrm{d}x$$

$$= -\frac{xe^{-ax}}{a}\Big|_0^\infty + \frac{1}{a}\int_0^\infty e^{-ax}\mathrm{d}x = 0 - \frac{e^{-ax}}{a^2}\Big|_0^\infty = \frac{1}{a^2}$$