THE CHEMIST'S TOOLKIT 12 Series expansions

A function $f(x)$ can be expressed in terms of its value in the vicinity of $x = a$ by using the **Taylor series**

$$f(x)=f(a)+\left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_a(x-a)+\frac{1}{2!}\left(\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right)_a(x-a)^2+\cdots$$
$$=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\mathrm{d}^n f}{\mathrm{d}x^n}\right)_a(x-a)^n \qquad \text{Taylor series} \qquad (12.1)$$

where the notation $(\ldots)_a$ means that the derivative is evaluated at $x = a$ and $n!$ denotes a **factorial** defined as

$$n! = n(n-1)(n-2)\ldots1, \quad 0! \equiv 1 \qquad \text{Factorial} \qquad (12.2)$$

The **Maclaurin series** for a function is a special case of the Taylor series in which $a = 0$. The following Maclaurin series are used at various stages in the text:

$$(1+x)^{-1}=1-x+x^2-\cdots=\sum_{n=0}^{\infty}(-1)^n x^n \qquad (12.3a)$$

$$\mathrm{e}^x=1+x+\tfrac{1}{2}x^2+\cdots=\sum_{n=0}^{\infty}\frac{x^n}{n!} \qquad (12.3b)$$

$$\ln(1+x)=x-\tfrac{1}{2}x^2+\tfrac{1}{3}x^3-\cdots=\sum_{n=1}^{\infty}(-1)^{n+1}\frac{x^n}{n} \qquad (12.3c)$$

Series expansions are used to simplify calculations, because when $|x| \ll 1$ it is possible, to a good approximation, to terminate the series after one or two terms. Thus, provided $|x| \ll 1$,

$$(1+x)^{-1} \approx 1-x \qquad (12.4a)$$

$$\mathrm{e}^x \approx 1+x \qquad (12.4b)$$

$$\ln(1+x) \approx x \qquad (12.4c)$$

A series is said to **converge** if the sum approaches a finite, definite value as n approaches infinity. If the sum does not approach a finite, definite value, then the series is said to **diverge**. Thus, the series expansion of $(1+x)^{-1}$ converges for $|x| < 1$ and diverges for $|x| \geq 1$. Tests for convergence are explained in mathematical texts.