CHEM1047 - Week 9 Lecture 2 - Integration, Part I

☐ *Chapters 23-25 of Monk and Munro, "Maths for Chemistry", 2nd edition.*

☐ *Chapter 6 of Steiner, "The Chemistry Maths Book", 2nd edition.*

Unlike differentiation, finding indefinite integrals is not a mechanical process – a finite algorithm that would be able to integrate an arbitrary function does not actually exist. In practice this means that experience and creativity can assist significantly in the integration process. At the most basic level, a table of indefinite integrals may be assembled by listing the functions that have the desired derivatives:

$\frac{df(x)}{dx}$	$f(x)$	$\int f(x)dx$
nx^{n-1}	x^n	$\frac{1}{n+1}x^{n+1}+C$
e^x	e^x	e^x+C
$\frac{1}{x}$	$\ln x$	$x\ln x-x+C$
$-\sin x$	$\cos x$	$\sin x+C$
$\cos x$	$\sin x$	$-\cos x+C$
$-\frac{1}{x^2}$	$\frac{1}{x}$	$\ln x+C$

However, this is not sufficient when combinations of elementary functions occur under the integral. Some basic techniques for dealing with those cases are reviewed in this lecture.

1. Constants added to the integration variable

Because adding an arbitrary constant k does not change the differential of the variable

$$d(x+k)=dx \tag{1}$$

the formulas for indefinite integrals of functions with a constant added to the argument are exactly the same as those for the variable without the constant:

$$\int f(x+k)dx=F(x+k)+C \tag{2}$$

Examples:

$$\int\frac{1}{x+2}dx=\ln(x+2)+C,\qquad \int\cos\left(x-\sqrt{3}\right)dx=\sin\left(x-\sqrt{3}\right)+C$$

2. Multiples of the integration variable

A frequently encountered situation is when a coefficient is present in front of the argument of a function that can be integrated by the rule table:

$$\int f(kx)dx=\frac{1}{k}F(kx)+C \tag{3}$$

This integral may be taken by a variable substitution $y = kx$, but the formula above provides a convenient shorthand – it is easy to demonstrate by differentiation that a coefficient of $1/k$ simply appears in front. Note that this also applies to the minus sign (in which case $k = -1$). Examples:

$$\int \cos(8x)\,dx = \frac{1}{8}\sin(8x) + C, \qquad \int \frac{1}{kx+1}\,dx = \frac{1}{k}\ln(kx+1) + C$$

3. Trigonometric power reduction and product-to-sum formulas

The following relations are useful for transforming products of trigonometric functions into their sums:

$$\cos^2(x) = \frac{1}{2}\left[1+\cos(2x)\right], \quad \sin^2(x) = \frac{1}{2}\left[1-\cos(2x)\right], \quad \sin(x)\cos(x) = \frac{1}{2}\sin(2x)$$
$$\sin(x)\sin(y) = \frac{1}{2}\left[\cos(x-y)-\cos(x+y)\right]$$
$$\cos(x)\cos(y) = \frac{1}{2}\left[\cos(x-y)+\cos(x+y)\right] \tag{4}$$
$$\sin(x)\cos(y) = \frac{1}{2}\left[\sin(x-y)+\sin(x+y)\right]$$

In the general case, the easiest way of integrating a complicated trigonometric expression is to convert all trigonometric functions to complex exponentials using Euler's formulas, where $i^2 = -1$:

$$e^{ix} = \cos(x) + i\sin(x), \qquad \cos(x) = \frac{e^{ix}+e^{-ix}}{2}, \qquad \sin(x) = \frac{e^{ix}-e^{-ix}}{2i} \tag{5}$$

Example:

$$\int \sin(2x)\sin(4x)\,dx = \frac{1}{2}\int\left[\cos(2x)-\cos(6x)\right]dx = \frac{\sin(2x)}{4} - \frac{\sin(6x)}{12} + C$$

4. Common trigonometric substitutions

The table below provides a few common rules (many more exist) of variable substitution for integrals containing common types of sub-expressions.

Sub-expression	Example	Substitution
$a^2 - x^2$	$\int \frac{dx}{\sqrt{a^2-x^2}}$	$x = a\sin(\varphi), \quad dx = a\cos(\varphi)\,d\varphi$
$a^2 + x^2$	$\int \frac{dx}{a^2+x^2}$	$x = a\tan(\varphi), \quad dx = a\sec^2(\varphi)\,d\varphi$
$f(\sin(x))\cos(x)$	$\int f(\sin(x))\cos(x)\,dx$	$y = \sin(x), \quad dy = \cos(x)\,dx$
$f(\cos(x))\sin(x)$	$\int f(\cos(x))\sin(x)\,dx$	$y = \cos(x), \quad dy = -\sin(x)\,dx$

Example:

$$\int \frac{dx}{4+x^2} = \begin{bmatrix} x = 2\tan\varphi \\ dx = \left[2/\cos^2(\varphi)\right]d\varphi \end{bmatrix} = \int \frac{2}{\cos^2(\varphi)}\frac{d\varphi}{4+4\sin^2(\varphi)/\cos^2(\varphi)} =$$
$$= \int \frac{2\,d\varphi}{4\cos^2(\varphi)+4\sin^2(\varphi)} = \frac{1}{2}\int d\varphi = \frac{\varphi}{2} + C = \frac{1}{2}\arctan\left(\frac{x}{2}\right) + C$$

5. Integration of separable fractions

For expressions of the type $P(x)/Q(x)$ where $P(x)$ and $Q(x)$ are polynomials and the degree of $P(x)$ is smaller than the degree of $Q(x)$ and

$$Q(x)=\prod_{k=1}^{n}(x-\alpha_k) \tag{6}$$

the following expansion is possible:

$$\frac{P(x)}{Q(x)}=\sum_{k=1}^{n}\frac{c_k}{x-\alpha_k} \tag{7}$$

That may be integrated directly. Example:

$$\int\frac{dx}{(x-1)(x+2)}=\int\left[\frac{a}{x-1}+\frac{b}{x+2}\right]dx$$

$$a(x+2)+b(x-1)=1 \quad\Rightarrow\quad \begin{cases}a+b=0\\2a-b=1\end{cases} \quad\Rightarrow\quad \begin{cases}a=+1/3\\b=-1/3\end{cases}$$

$$\int\frac{dx}{(x-1)(x+2)}=\frac{1}{3}\int\left[\frac{1}{x-1}-\frac{1}{x+2}\right]dx=\frac{1}{3}\left[\ln(x-1)-\ln(x+2)\right]+C$$

6. Parametric differentiation

If a function $f(x,a)$ depends on a parameter a and both $f(x,a)$ and $f'_a(x,a)$ are continuous, then the differentiation operation with respect to a and the integration operation with respect to x can be performed in any order:

$$\frac{\partial}{\partial a}\int f(x,a)\,dx=\int\left[\frac{\partial}{\partial a}f(x,a)\right]dx \tag{8}$$

Example:

$$\int xe^{ax}dx=\int\left[\frac{\partial}{\partial a}e^{ax}\right]dx=\frac{\partial}{\partial a}\int e^{ax}dx+C=\frac{\partial}{\partial a}\left[\frac{e^{ax}}{a}\right]+C=\frac{axe^{ax}-e^{ax}}{a^2}+C$$

7. Integration of power series

Taylor series may be differentiated and integrated term by term. Note that the convergence radius may change. Examples:

$$\left[\sin(x)\right]'=\left[\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k+1}}{(2k+1)!}\right]'=\sum_{k=0}^{\infty}\frac{(-1)^k(2k+1)x^{2k}}{(2k+1)!}=\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k}}{(2k)!}=\cos(x)$$

$$\int\cos(x)\,dx=\int\left[\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k}}{(2k)!}\right]dx=\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k)!}\int x^{2k}dx=\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k+1}}{(2k+1)!}+C=\sin(x)+C$$