

TABLE OF USEFUL INTEGRALS FOR QUANTUM CHEMISTRY

Indefinite forms:

$$\int x^n dx = \frac{x^{n+1}}{n+1} + C$$

$$\int \frac{1}{x} dx = \ln x + C$$

$$\int u dv = uv - \int v du$$

$$\int \sin(ax) dx = -\frac{1}{a} \cos(ax) + C$$

$$\int \cos(ax) dx = \frac{1}{a} \sin(ax) + C$$

$$\int \sin^2(ax) dx = \frac{1}{2}x - \frac{1}{4a} \sin(2ax) + C$$

$$\int \cos^2(ax) dx = \frac{1}{2}x + \frac{1}{4a} \sin(2ax) + C$$

$$\int x \sin(ax) dx = \frac{1}{a^2} \sin(ax) - \frac{x}{a} \cos(ax) + C$$

$$\int x \cos(ax) dx = \frac{1}{a^2} \cos(ax) + \frac{x}{a} \sin(ax) + C$$

$$\int x \sin^2(ax) dx = \frac{x^2}{4} - \frac{x \sin(2ax)}{4a} - \frac{\cos(2ax)}{8a^2} + C$$

$$\int x \cos^2(ax) dx = \frac{x^2}{4} + \frac{x \sin(2ax)}{4a} + \frac{\cos(2ax)}{8a^2} + C$$

$$\int x^2 \sin^2(ax) dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3} \right) \sin(2ax) - \frac{x \cos(2ax)}{4a^2} + C$$

$$\int x^2 \cos^2(ax) dx = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3} \right) \sin(2ax) + \frac{x \cos(2ax)}{4a^2} + C$$

$$\int x^m e^{ax} dx = \frac{x^m e^{ax}}{a} - \frac{m}{a} \int x^{m-1} e^{ax} dx + C$$

$$\int x e^{ax} dx = \frac{e^{ax}}{a^2} (ax - 1)$$

$$\int \sin(ax) \sin(bx) dx = \frac{\sin(a-b)x}{2(a-b)} - \frac{\sin(a+b)x}{2(a+b)} + C \quad \text{if } a^2 \neq b^2$$

$$\int \frac{e^{ax}}{x^m} dx = -\frac{1}{m-1} \frac{e^{ax}}{x^{m-1}} + \frac{a}{m-1} \int \frac{e^{ax}}{x^{m-1}} dx + C$$

Definite Forms:

$$\int_0^{\pi} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = \int_0^{\pi} \cos\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) dx = \frac{a}{2} \delta_{nm}$$

$$\int_0^{\pi} x \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^2}{4}$$

$$\int_0^{\pi} \sin\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) dx = 0$$

$$\int_0^{\pi} \sin^2(mx) dx = \int_0^{\pi} \cos^2(mx) dx = \frac{\pi}{2}$$

$$\int_0^{\pi} \frac{\sin x}{\sqrt{x}} dx = \int_0^{\pi} \frac{\cos x}{\sqrt{x}} dx = \sqrt{\frac{\pi}{2}}$$

$$\int_0^{\pi} x^n e^{-ax} dx = \frac{n!}{a^{n+1}} \quad (a > 0, n \text{ positive integer})$$

$$\int_0^{\pi} x^{2n} e^{-ax} dx = \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}} \quad (a > 0, n \text{ positive integer})$$

$$\int_0^{\pi} x^{2n+1} e^{-ax} dx = \frac{n!}{2a^{n+1}} \quad (a > 0, n \text{ positive integer})$$

$$\int_0^{\pi} e^{-ax^2} dx = \sqrt{\frac{\pi}{4a}}$$



Quantum Chemistry Integrals And Tables

Jicheng Xie



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