常用公式

$$\sin 2A = 2\sin A\cos A$$

$$\cos 2A = \cos^2 A - \sin^2 A$$

$$\tan 2A = \frac{2\tan A}{1-\tan^2 A}$$

$$\sin\frac{A}{2} = \pm\sqrt{\frac{1-\cos A}{2}}$$

$$\cos\frac{A}{2} = \pm\sqrt{\frac{1+\cos A}{2}}$$

$$\tan\frac{A}{2} = \pm\sqrt{\frac{1-\cos A}{1+\cos A}} = \frac{\sin A}{1+\cos A}$$

$$\sin^2 A = \frac{1}{2} - \frac{1}{2}\cos 2A$$

$$\cos^2 A = \frac{1}{2} + \frac{1}{2}\cos 2A$$

$$\sin A\sin B = \frac{1}{2}\left[\cos(A-B) - \cos(A+B)\right]$$

$$\cos A\cos B = \frac{1}{2}\left[\cos(A-B) + \cos(A+B)\right]$$

$$\sin A\cos B = \frac{1}{2}\left[\sin(A-B) + \sin(A+B)\right]$$

$$\int x\sin^2 ax\,dx = \frac{x^2}{4} - \frac{x\sin 2ax}{4a} - \frac{\cos 2ax}{8a^2}$$

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

$$\int_0^\infty x^n e^{-ax}dx = \frac{n!}{a^{n+1}}$$

$$\int_0^\infty e^{-ax^2}dx = \left(\frac{\pi}{4a}\right)^{1/2}$$

$$\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{1 \bullet 3 \bullet 5 \cdots (2n-1)}{2^{n+1} a^n} \left(\frac{\pi}{a} \right)^{1/2}$$

$$\int_0^\infty x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}}$$

物理常數

$N_A = 6.02214 \times 10^{23}$ mol^{-1}

amu = 1.66054×10^{-27} kg

$a_0 = 5.29177 \times 10^{-11}$ m

$k_B = 1.38065 \times 10^{-23}$ J K^{-1}

$m_e = 9.10938 \times 10^{-31}$ kg

$m_p = 1.67262 \times 10^{-27}$ kg

$m_n = 1.67493 \times 10^{-27}$ kg

R = 8.31447 J K^{-1} mol^{-1}

$4\pi\varepsilon_0 = 1.11265\ 10^{-10}$ C^2 J^{-1} m^{-1}

$h = 6.62608 \times\ 10^{-34}$ J s

e = $1.602176 \times\ 10^{-19}$ C

c = 2.99792458×10^8 m s^{-1}

1 joule = 4.184 cal

1 eV = 96.4853 kJ/mol = 23.0605 kcal/mol

1 cm^{-1} = 1.196266×10^{-2} kJ/mol = 2.8591×10^{-3} kcal/mol

1 Hartree = 2625.50 kJ/mol = 627.5095 kcal/mol