Atomic Units and other units, Conversion Factors:

Fundamental quantities

m = 9.109534 $\times 10^{-28}$ g

e = 1.60217733 $\times 10^{-19}$ C = 4.803242$\times 10^{-10}$ esu

c = 2.99792458$\times 10^{10}$ cm sec^{-1}

h = 6.626176 $\times 10^{-27}$ erg sec

N_{Avo} = 6.022045 $\times 10^{23}$ mole^{-1}

$\hbar$ = 1.0545887 $\times 10^{-27}$ erg sec = 1.054592 $\times 10^{-34}$ J sec

k_B = 1.380662 $\times 10^{-16}$ erg K^{-1} = 1.380662 $\times 10^{-23}$ J K^{-1}

a_0 = 5.29177249$\times 10^{-11}$ m

C means Coulomb, c means speed of light

Atomic Units (au)

distance, r	$a_0 \equiv \hbar^2/me^2$	bohr	
energy, V	$E_h = e^2/a_0$	hartree	1 hartree= 4.3597$\times 10^{-18}$ J
electric dipole moment, μ	ea_0		
electric quadrupole moment, Q_2	ea_0^2		
electric octopole moment, Q_3	ea_0^3		
electric hexadecapole moment, Q_4	ea_0^4		
electric dipole polarizability, α	$e^2a_0^2 E_h^{-1}$		
dispersion coefficient C_6	$E_h a_0^6$	hartree bohr^6	
force constant, $(\partial^2V/\partial r^2)$	$E_h a_0^{-2}$	hartree bohr^{-2}	1 hartree bohr^{-2} = 15.569141 mdyne Å^{-1}
force constant, $(\partial^2V/\partial \theta^2)$	$E_h a_0^{-2}$	hartree rad^{-2}	1 hartree rad^{-2} = 4.3598 mdyne Å

Other units and Conversions:

1 hartree	4.3597×10^{-11} erg	4.3597×10^{-18} J	27.212 eV
1 Å	0.1 nm	10^{-10} m	1.889726 bohr
1 bohr	0.529177249 Å		
1 hartree bohr^{-2}	15.569141 mdyn Å^{-1}		
mdyn Å^{-1}	10^2 N m^{-1}	10^2 J m^{-2}	
1 joule	m^2 kg s^{-2}		
1 newton	m kg s^{-2}	J m^{-1}	
1 esu	10/c C	3.3356×10^{-10} C	
debye	1 esu Å	3.3356×10^{-30} C m	
1 erg = 10^{-7} J	q^2/r	1 esu^2 cm^{-1}	
1 joule	$q^2/[4\pi\varepsilon_0 r]$	$(1/1.1127\times10^{-10})$ C^2 m^{-1}	
1 erg	1 gauss^2 cm^3		
1 amagat	2.687×10^{19} molecules cm^{-3}		
mean square torque, $\langle C^2\rangle/\rho$, (cm^{-1})^2 amagat^{-1}	$(\partial V/\partial\theta)^2$ in (energy/rad)^2 r^2dr in (distance)^3	convert energy^2 to (cm^{-1})^2, (distance)^3 to cm^3	multiply integral by 6.022045×10^{23} / 22414 cm^3
Bohr magneton, μ_B	$e\hbar/2mc$	9.27408×10^{-21} erg G^{-1}	9.27408×10^{-21} G cm^3
nuclear magneton, μ_N	$e\hbar/2m_pc$	5.05082×10^{-24} erg G^{-1}	
μ_B B, B in Gauss	9.27408×10^{-21} B erg		
μ_B r^{-3}, r in cm	9.27408×10^{-21} r^{-3} G		
1 joule = 10^7 erg	7.2429×10^{22} K	6.24146×10^{18}eV	5.03404×10^{22} cm^{-1}
1eV	1.6021892×10^{-19} J	8065.48 cm^{-1}	1.1605×10^4 K
1 hartree	27.212 eV	4.3597×10^{-18} J	3.1577×10^5 K
1 cm^{-1}	1.4388 K	1.23985×10^{-4} eV	1.98648×10^{-23} J

List of possibly useful integrals

$\int \sin(ax)dx = -(1/a)\cos(ax)$
$\int \cos(ax)dx = (1/a)\sin(ax)$
$\int \sin^2(ax)dx = ½\ x - (1/4a)\sin(2ax)$
$\int \sin^4(ax)dx = 3x/8 - (1/4a)\sin(2ax) + (1/32a)\sin(4ax)$
$\int \cos^2(ax)dx = ½\ x + (1/4a)\sin(2ax)$
$\int \cos^4(ax)dx = 3x/8 + (1/4a)\sin(2ax) + (1/32a)\sin(4ax)$
$\int \sin(ax)\sin(bx)dx = [1/2(a-b)]\sin[(a-b)x)] - [1/2(a+b)]\sin[(a+b)x)], \quad a^2 \neq b^2$
$\int \cos(ax)\cos(bx)dx = [1/2(a-b)]\sin[(a-b)x)] + [1/2(a+b)]\sin[(a+b)x)], \quad a^2 \neq b^2$
$\int x \sin(ax)dx = (1/a^2)\sin(ax) - (x/a)\cos(ax)$
$\int x \cos(ax)dx = (1/a^2)\cos(ax) + (x/a)\sin(ax)$
$\int x^2 \cos(ax)dx = [(a^2x^2 - 2)/a^3]\sin(ax) + 2x\cos(ax)/a^2$
$\int x^2 \sin(ax)dx = -[(a^2x^2 - 2)/a^3]\cos(ax) + 2x\sin(ax)/a^2$
$\int x \sin^2(ax)dx = x^2/4 - x\sin(2ax)/4a - \cos(2ax)/8a^2$
$\int x^2 \sin^2(ax)dx = x^3/6 - [x^2/4a - 1/8a^3]\sin(2ax) - x\cos(2ax)/4a^2$
$\int x \cos^2(ax)dx = x^2/4 + x\sin(2ax)/4a + \cos(2ax)/8a^2$
$\int x^2 \cos^2(ax)dx = x^3/6 + [x^2/4a - 1/8a^3]\sin(2ax) + x\cos(2ax)/4a^2$
$\int x \exp(ax)dx = \exp(ax)\ (ax-1)/a^2$
$\int x \exp(-ax)dx = \exp(-ax)\ (-ax-1)/a^2$
$\int x^2 \exp(ax)dx = \exp(ax)\ [x^2/a - 2x/a^2 + 2/a^3]$
$\int x^m \exp(ax)dx = \exp(ax) \sum_{r=0 \text{ to } m} (-1)^r\ m!x^{m-r}/(m-r)!a^{r+1}$
$\int dx/x(a+bx) = -(1/a)\ln[(a+bx)/x]$

$\int_0^\infty x^n \exp(-ax)dx = n!/a^{n+1}$ $\quad a > 0$, n positive integer
$\int_0^\infty x^2 \exp(-ax^2)dx = (1/4a)(\pi/a)^{½}$ $\quad a > 0$
$\int_0^\infty x^{2n} \exp(-ax^2)dx = (1\cdot3\cdot5\cdot\ldots\cdot(2n-1)/(2^{n+1}a^n)(\pi/a)^{½}$ $\quad a > 0$
$\int_0^\infty x^{2n+1} \exp(-ax^2)dx = n!/2a^{n+1}$ $\quad a > 0$, n positive integer
$\int_0^\infty \exp(-a^2x^2)dx = (1/2a)\ (\pi)^{½}$ $\quad a > 0$
$\int_0^\infty \exp(-ax)\cos(bx)dx = a/(a^2+b^2)$ $\quad a > 0$
$\int_0^\infty \exp(-ax)\sin(bx)dx = b/(a^2+b^2)$ $\quad a > 0$
$\int_0^\infty x\exp(-ax)\sin(bx)dx = 2ab/(a^2+b^2)^2$ $\quad a > 0$
$\int_0^\infty x\exp(-ax)\cos(bx)dx = (a^2-b^2)/(a^2+b^2)^2$ $\quad a > 0$
$\int_0^\infty \exp(-a^2x^2)\cos(bx)dx = [(\pi)^{½}/2a]\cdot\exp[-b^2/4a^2]$ $\quad ab \neq 0$

Some useful identities:

$\sin(2x) = 2\sin x \cos x \qquad \cos(2x) = \cos^2x - \sin^2x = 2\cos^2x - 1$

$e^{ix} = \cos x + i\sin x; \quad e^{-ix} = \cos x - i\sin x; \qquad$ from which, $\quad \cos x = ½\{e^{ix} + e^{-ix}\}$