

**Appendix 2:****Conversion Factors and Fundamental Constants.**

Electron mass	= $9.10953 \times 10^{-31}$ kg
1 Atomic mass unit	= 1822.8880 Electron mass
1 Electron volt (e V)	= $1.60218 \times 10^{-19}$ J
	= 96.485 kJ mol <sup>-1</sup>
	= 23.06035 kcal mol <sup>-1</sup>
	= 8065.5 cm <sup>-1</sup>
1 Hartree	= 627.32 kcal mol <sup>-1</sup>
	= 27.2116 e V
1 Angstrom (Å)	= $10^{-10}$ m
1 cm <sup>-1</sup>	= $1.9864 \times 10^{-23}$ J
1 Bohr (a <sub>0</sub> )	= $5.29177 \times 10^{-11}$ m
1 atomic mass unit	= $1.6605402 \times 10^{-27}$ kg
Velocity of light (c)	= $2.997925 \times 10^8$ m s <sup>-1</sup>
Boltzmann constant (k)	= $1.38 \times 10^{-23}$ J K <sup>-1</sup>
Gas constant (R)	= 8.31447 J K <sup>-1</sup> mol <sup>-1</sup>
Plank constant (h)	= $6.62608 \times 10^{-34}$ J s
Avogadro's constant (N <sub>A</sub> )	= $6.0221367 \times 10^{23}$ mol <sup>-1</sup>
1 Electron Charge (e)	= $4.803242 \times 10^{-10}$ esu
	= $1.602188 \times 10^{-19}$ Coulomb