

## Atomic Units

Since 1960 the international scientific community has agreed on an "official" set of basic units for all measurements, *Le Système International d'Unités*, or SI for short.

See website maintained by the National Institute of Standards and Technology (NIST):

<http://physics.nist.gov/cuu/Units/introduction.html>

## AU-2

Seven defined SI units:

meter (m), kilogram (kg), second (s), ampere (A),  
kelvin (K), mole (mol) and candela (cd).

Also many defined SI units such as the Joule (J), Pascal (Pa), etc. as well as myriad non-SI units such as inches, etc.

In molecular/atomic QM we often use atomic units to give the electronic Schrödinger a simple appearance

## AU-3

In atomic units, the unit of mass is the rest mass of an electron ( $m_e$ ); the unit of charge is the elementary charge ( $e$ ); the unit of distance is the radius of the first bohr orbit ( $a_0$ ), and the unit of energy is taken to be the hartree:  $e^2/4\pi\epsilon_0 a_0$

## AU-4

Quantity	Atomic Unit	SI Equivalent
Mass	$m_e = 1$	$9.10913897 \times 10^{-34} \text{ kg}$
Charge	$e = 1$	$1.60217733 \times 10^{-19} \text{ C}$
Length	$a_0 = 1 \text{ bohr}$	$0.529177249 \times 10^{-10} \text{ m}$
Energy	hartree	$4.35974823 \times 10^{-18} \text{ J}$ $27.211396 \text{ eV}$
Ang. mom.	$\hbar/2\pi = 1$	$1.05457266 \times 10^{-34} \text{ Js}$