Atomic Units and Their SI Equivalents

We will for the most part use SI units in this course. However, be aware that many graduate texts still use the gaussian unit system, because the electromagnetic field equations are somewhat more symmetric than in SI units. A third system of units is also useful—from time to time, we will lapse into the "theorist's units" appropriate to atomic physics, making many uninteresting constants disappear by setting them equal to unity.

The system of atomic units is defined by the following (dimensions given in square brackets):

$\hbar = 1$ [E ·t or m ℓ^2 t^{-1}] $\qquad$ $4\pi\varepsilon_0 = 1$

$m_e = 1$ [m] $\qquad$ $\dfrac{4\pi}{\mu_0} = c^2 = 1/\alpha^2$

$e = 1$ [$m^{1/2}$ $\ell^{3/2}$ t^{-1}]

The atomic units for other common physical quantities are given below:

Quantity	**Unit** ($K \equiv 1/4\pi\varepsilon_0$)	**SI equivalent**	**Name or Description**
Charge	$e = 1$	1.602×10^{-19} C	electron charge
Angular Momentum	$\hbar = 1$	1.05×10^{-34} J·sec	"h-bar"
Mass	$m_e = 1$	9.11×10^{-31} kg	electron mass
Length	$a_0 = \dfrac{\hbar^2}{m_e K e^2} = 1$	5.29×10^{-11} m	Bohr or "atomic unit"
Velocity	$Ke^2/\hbar = c\alpha = 1$	2.188×10^{6} m/sec	velocity in first Bohr orbit
Time	$\dfrac{\hbar^3}{m_e K^2 e^4} = 1$	2.419×10^{-17} s	$1/\omega$ for first Bohr orbit
Energy	$m_e K^2 e^4/\hbar^2 = 1$	4.36×10^{-18} J, or 219474 cm^{-1}	Hartree (= 2 Rydbergs)
Magnetic moment	$\mu_B = \dfrac{e\hbar}{2m_e} = 1/2$	1.400×10^{10} Hz/Tesla (times h) or 1.400 MHz/gauss	Bohr magneton
Electric field	$Ke/a_0^2 = 1$	5.142×10^{11} V/m	Internal field of H atom

The fine structure constant is given by $\alpha = \dfrac{Ke^2}{c\hbar} = 1/137.036$, so in atomic units, the speed of light is $c = 1/\alpha$.

Also very useful: The wavenumber or "inverse centimeter" is very often used as an energy unit in spectroscopy; what one means by this is:

$1\ \text{cm}^{-1} = hc/\lambda$ with $\lambda = 1$ cm
$= 1.98658 \times 10^{-23}$ J
$= 2.99792458 \times 10^{10}$ Hz (exactly)
$= 1/8065.02$ eV