

Atomic Units

You may have noticed that the energies of the hydrogen atom involve lots of constants:

$$E_n = \frac{-Z^2 \mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \times \frac{1}{n^2}$$

All of these constants become cumbersome when one does computations. For this reason, a more convenient system of units was defined for working with atoms and molecules. These units are called *atomic units*. When one works in atomic units, lots of coefficients turn into 1! For example, the Schrödinger equation for a hydrogenic atom becomes (assuming infinite nuclear mass; i.e., $\mu = m_e$)

$$\left(-\frac{1}{2} \nabla^2 - \frac{Z}{r}\right) \psi = E \psi$$

and the energies become

$$E_n = \frac{-Z^2}{2n^2}$$

The ground-state wave function is

$$\psi_{1s} = \left\{ \frac{Z^3}{\pi} \right\}^{0.5} e^{-Zr}$$

Some of the problems we work will refer to atomic units, and they will be easier to handle that way. Furthermore, you may run across atomic units in the future, so it is helpful to be introduced to them. The funny thing about atomic units is that the unit is designated "a.u." regardless of whether it refers to energy, mass, length, time, etc. (sometimes for clarity we speak, for example, of "atomic time units"). It is up to you to keep track of whether a quantity is of energy, mass, etc. If you work in atomic units, you should express all quantities in atomic units.

Some common quantities in the usual units and in atomic units are:

mass	$m_e = 9.109534 \times 10^{-31} \text{ kg}$	1 a.u. = mass of electron
length	$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} = 5.292 \times 10^{-11} \text{ m}$ "one bohr"	1 a.u. = most probable distance of 1s electron from nucleus of H atom
time	$\tau_0 = \frac{a_0 \hbar}{e^2} = 2.4189 \times 10^{-17} \text{ sec}$	1 a.u. = time for 1s electron in H atom to travel one bohr
charge	$e = 1.602177 \times 10^{-19} \text{ C}$	1 a.u. (Note that charge of electron = -1 a.u.)
energy	$\frac{e^2}{4\pi\epsilon_0 a_0} = 4.359814 \times 10^{-18} \text{ J}$	1 a.u., also known as a "Hartree" (Note that total energy of 1s electron in H atom = $-\frac{1}{2}$ a.u.)

Over

angular momentum $\hbar = 1.0545887 \times 10^{-34} \text{ J sec}$ 1 a.u. (angular momentum for particle in ring = 0,1,2...a.u.)

electric field strength $\frac{e}{a_0^2} = 5.1423 \times 10^9 \text{ V/cm}$ 1 a.u. = electric field strength at distance of 1 bohr from proton

permittivity $4\pi\epsilon_0 = 1.11265 \times 10^{10} \text{ J}^{-1}\text{C}^2\text{m}^{-1}$ 1 a.u. = permittivity of vacuum

Note one ambiguity: the "atomic mass unit" or "amu" is not part of this system. An amu has the symbol u and is equal to $1.66054 \times 10^{-27} \text{ kg}$ (whereas 1 a.u. of mass, as listed above, is equivalent to $9.109534 \times 10^{-31} \text{ kg}$, the mass of an electron). The nice thing about the amu is that the mass of a single atom is its atomic mass number times one amu. For example, the mass of a carbon atom is 12.01 amu or $12.01 \times (1.66054 \times 10^{-27} \text{ kg}) = 1.994 \times 10^{-26} \text{ kg}$.