

Atomic units $\hbar = m = e = 1$ (a.u.) (The units in the electron's world.)

Length= a_0 = Bohr radius= **0.528×10^{-8} cm**

Velocity= v_0 =electron velocity in 1st Bohr orbit= **$\alpha c = 2.18 \times 10^8$ cm/s**

Energy= twice of ionization potential of H=**27.21 eV** (called Hartree by chemists)

Time= $a_0/v_0 = 2.42 \times 10^{-17}$ sec= **24.2 as** (1fs= 41 a.u)

units of frequency= $v_0/a_0 = 4.13 \times 10^{16}$ sec⁻¹

Electric field = $e/a_0^2 = 5.14 \times 10^9$ V/cm

Other units:

One atomic unit of magnetic field is defined for a Bohr magneton in a B field which has the energy of 13.6 eV. Or $\mu_B B = 13.6 \text{ eV}$ where $\mu_B = e\hbar / 2mc = 5.788 \times 10^{-5} \text{ eV / Tesla}$

Thus 1 a.u. of magnetic field = **2.35×10^5 Tesla**

Laser intensity= $\frac{1}{2} \epsilon_0 c E^2 = 3.51 \times 10^{16} \text{ W/cm}^2$ for **peak** E field at 1 a.u.

Energy conversion factors

1 eV = 8065.54 **cm⁻¹**

1 a.u = 27.211396 eV = 219 474.63 05 **cm⁻¹** = 2 Ry

1 Ry = 13.6057 eV

1 degree **kelvin** = 0.0862 meV (energy units for cold atoms)
= 0.695 **cm⁻¹**

1 **Kcal/mol**= 0.0434 eV = 43.4 meV (energy units used by chemists)

1 **GHz** $\rightarrow 6.6 \times 10^{-7}$ eV (energy units by laser physicists)

(be careful here-- GHz is the frequency f , to get the energy you need the conversion $\omega = 2\pi f$ to get it right. Thus $2\pi \times 4.13 \times 10^{16} \text{ Hz} \rightarrow 27.21 \text{ eV}$)

Frequently used constants

Speed of light in vacuum $c = 2.997\,924\,580 \times 10^8$ m/s (exact-by definition)

Planck's constant, $h = 6.6260755 \times 10^{-34}$ J-s = 4.136×10^{-15} eV-s

electron charge $q = 1.60217733 \times 10^{-19}$ coulomb

Avogadro number= 6.022×10^{23} /mole

Boltzmann's constant $k = 1.380658 \times 10^{-23}$ J/K = 8.617×10^{-5} eV/K

Short-hand notations.

10^9 =giga, 10^{12} =tera; 10^{15} =**peta**; 10^{18} =exa; 10^{21} =zetta; 10^{24} =yocto

10^{-9} =nano 10^{-12} =pico; 10^{-15} =femto; 10^{-18} =**atto**; 10^{-21} =zepto; 10^{-24} =yotta

Notable wavelengths, frequencies and energies

photon wavelength to ionize H: 911 °A

Lyman- α of H: 1216 °A $\rightarrow$ 10.2 eV or 1 nm $\rightarrow$ 1.24 keV

photon momentum (a.u.) $k = 2.7 \times 10^{-4} E$ (eV)

de Broglie wavelength for **electron**, 100 eV is **1.22** angstrom

Lasers

For $\lambda = 1$ °A, photon energy= 455.71 au for 800 nm $\rightarrow \omega = 0.057 au$

laser peak intensity (linear polarized) = 3.5×10^{16} W/cm²

$$U_p = E^2 / 4 \omega^2 = 9.33 I (10^{14} \text{ W/cm}^2) \lambda^2 (\text{in } \mu\text{m})$$

(6eV for 800 nm at 10^{14} W/cm²)

Keldysh parameter $\gamma = \sqrt{I / (2U_p)}$

time-frequency width relation for a chirped pulse: $\Delta\omega = \frac{4 \ln 2}{\tau_x} \sqrt{1 + \xi^2}$

Gaussian pulse

$$I(\omega) = e^{-\tau^2 (\omega - \omega_0)^2 / (4 \ln 2)} \quad E(t) = e^{-2 \ln 2 t^2 / \tau^2}$$

(τ is FWHM in time domain)

width in eV for a Gaussian pulse for $\tau = 1$ fs is 1.83 eV.

1.5. Oscillator strength and transition rates

$$A = 2 \cdot (\omega^2 / c^3) f \quad (4.13 \times 10^{16}) \quad 1/\text{sec}$$

where ω is in a.u. , $c=137.03604$ and f is the oscillator strength for emission