1 Atomic units

Hartree units are named after the physicist Douglas Hartree[1], in this unit *the numerical values of the following four fundamental physical constants are all unity by definition.* They are:

- **Reduced Planck Constant** $\hbar = 1$ (unit of action)
- **Elementary charge** $e = 1$ (unit of charge)
- **Bohr radius** $a_0 = 1$ (unit of length)
- **Electron mass** $m_e = 1$ (unit of mass)

Each unit in this system can be expressed as a product of powers of four physical constants *without a multiplying constant.* Therefore, they are consistent units, meaning that given any mathematical expression, if all the values are in atomic unit, the result will come out as atomic unit without the need for conversion. The derived units in atomic unit system are converted to SI unit by replacing the value of those constants (the constants are used as units).

Table 1: Defining constants

Symbol	**Definition**	**Value in SI units**
$\hbar$	$\hbar$	$1.054571 \times 10^{-34} J \cdot s$
e	e	$1.602176 \times 10^{-19} C$
a_0	$4\pi\epsilon_0\hbar^2/(m_e e^2)$	$5.291772 \times 10^{-11} m$
m_e	m_e	$9.109383 \times 10^{-31} kg$
E_h	$\hbar^2/(m_e a_0^2)$	$\hbar^2/(m_e a_0^2)$

2 Unit conversion

As an example, the speed of light in atomic unit of velocity is approximately 137.036, The atomic unit of velocity is expressed by the constants $a_0 E_h/\hbar$, which is converted to SI unit by $a_0 E_h/\hbar = 2.187 \times 10^6 m/s$, and therefore $137.036 \times 2.187 \times 10^6 = 2.99 \times 10^8 m/s$

Table 2: Derived atomic units

Atomic unit of	**Expression**	**Value in SI**
Action	$\hbar$	$1.054 \times 10^{-34} J \cdot s$
Charge	e	$1.602 \times 10^{-19} C$
Charge Density	e/a_0^3	$1.081 \times 10^1 2C \cdot m^{-3}$
Current	$eE_h/\hbar$	$6.623 \times 10^{-3} A$
Electric Field	$E_h/(ea_0)$	$5.142 \times 10^1 1V/m$
Electric Potential	E_h/e	$27.211V$
Electric Dipole moment	ea_0	$8.478 \times 10^{-30} C \cdot m$
Energy	E_h	$4.359 \times 10^{-18} J$
Force	E_h/a_0	$8.238 \times 10^{-8} N$
Length	a_0	$5.291 \times 10^{-11} m$
Magnetic Dipole Moment	$e\hbar/m_e$	$1.854 \times 10^{-23} J/T$
Mass	m_e	$9.109 \times 10^{-31} kg$
Momentum	$\hbar/a_0$	$1.992 \times 10^{-24} kg \cdot m/s$
Permitivity	$e^2/(a_0 E_h)$	$1.112 \times 10^{-10} F/m$
Time	$\hbar/E_h$	$2.418 \times 10^{-17} s$
Pressure	E_h/a_0^3	$2.942 \times 10^{13} Pa$
Velocity	$a_0 E_h/\hbar$	$2.187 \times 10^6 m/s$

[1] the reference of this note is Wikipedia