Atomic Units

Eliminate most physical constants from electronic-structure calculations

Unit of length – Bohr radius

$$a_0 = \frac{\hbar^2}{Me^2}$$

where M is the electron mass,
e the electron charge,
$\hbar$ Plancks constant $/2\pi$

$$a_0 \equiv 0.529177 \text{ Å}$$

Unit of energy – Twice the ionization energy of the H atom

$$e^2/a_0 \equiv 27.212 \ ev$$

Unit of mass – mass of electron