

Atomic Units

eliminate most physical constants from electronicstructure calculations.

Unit of length – Bohr radius

$$a_0 = \hbar^2 / (m_e e^2) = 0.529177 \text{ \AA}$$

where m_e is the electron mass,
 e the electron charge,
 \hbar Plancks constant / 2π

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

$$e^2 / a_0 = 27.212 \text{ eV}$$

Unit of mass – mass of electron (m_e)