Atomic units (a.u.)

1 a.u. of mass $= m_e = 9.109 \times 10^{-31}\, kg$

1 a.u. of charge = charge of a proton $= 1.602 \times 10^{-19}\, C$

1 a.u. of length $= 0.52918 \times 10^{-10}\, m = 0.52918$ Å

1 a.u. of energy $= 1\, hartree = 4.360 \times 10^{-18}\, J$
$= 27.211\, eV = 2625\, kJ/mol = 627.5\, kcal/mol$

1 a.u. of permittivity $= 4\pi\epsilon_0 = 1.113 \times 10^{-10}\, C^2\, J^{-1}\, m^{-1}$
therefore $U_{electrostatic} = Q_1 Q_2 / r$ in a.u.

1 a.u. of time $= 2.419 \times 10^{-17}\, s$

1 a.u. of action $= h/2\pi = \hbar = 1.0546 \times 10^{-34}\, J\, s$

1 a.u. of electric dipole $= 2.5412\, D = 2.5412$ Debye
$= 3.336 \times 10^{-30}\, C\, m$

k_B, RT when $T = 298\, K$:
$0.00094\, a.u. = 0.026\, eV = 0.59\, kcal/mol = 2.5\, kJ/mol$

Range for various types of interaction energies (approximate)

chemical bonds: $\approx$ 1 — 10 eV (20 — 200 kcal/mol)

molecule pair interactions in liquids: $\approx$ 1 — 5 kcal/mol

molecule pair interactions in gases: $\approx$ 0.1 — 1 kcal/mol

ionization energies: $\approx$ 4 — 20 eV

electron affinities: $\approx$ 0 — 4 eV