Contents

Units

Atomic units (a.u.) will be used throughout this monograph. They are such that $\hbar = \mathrm{m} = \mathrm{e} = 1$, where $\hbar$ is Planck's constant h divided by 2π, m is the mass of the electron and $-\mathrm{e}$ is the charge of the electron. Thus the atomic unit of length $a_0 = \hbar^2/\mathrm{me}^2 \approx 5.292 \times 10^{-9}$ cm, which is the radius of the first Bohr orbit of the hydrogen atom with infinite nuclear mass. Using this unit of length, collision cross sections, which have the dimension of an area, are then expressed, either in units of $a_0^2 \approx 2.800 \times 10^{-17}\,\mathrm{cm}^2$ or in units of $\pi a_0^2 \approx 8.797 \times 10^{-17}\,\mathrm{cm}^2$. The atomic unit of time is given by $\hbar^3/\mathrm{me}^4 = 2.419 \times 10^{-17}$ s, while the unit of velocity is $\mathrm{e}^2/\hbar = 2.188 \times 10^8\,\mathrm{cm\,s}^{-1}$. The atomic unit of energy is $\mathrm{e}^2/a_0 \approx 27.21$ eV, which is twice the ionization energy of the hydrogen atom in its ground state and twice the Rydberg unit of energy. The fine-structure constant $\alpha = \mathrm{e}^2/\hbar\mathrm{c} \approx 1/137$ is dimensionless, where c is the velocity of light in a vacuum.