

Constants and units

Table 9.1: Fundamental constants defining the atomic units.

Bohr radius	a_0	0.529 177 2083 D-10 m
Electron Mass	m_e	9.10938188D-31 kg
Action	\hbar	1.054 571 60D-34 J s
Electron charge	e	1.602 176 462D-19 C
Kelvin	K	
mole	mol	
radian	rad	

Table 9.2: A list of the universal constants in atomic units.

Hartree	E_h	$\hbar^2 a_0^{-2} m_e^{-1}$
Permittivity of vacuum	ϵ_0	$0.07957747154594767 e^2 a_0 m_e \hbar^{-2}$
Permeability of vacuum	μ_0	$0.0006691762496807159 a_0 m_e e^{-2}$
Impedance of vacuum	Z_0	$0.0917012364137738 \hbar e^{-2}$
Speed of light in vacuum	c_0	$137.0359996287515 \hbar a_0^{-1} m_e^{-1}$
Proton rest mass	m_p	$1836.152663302331 m_e$

Neutron rest mass	m_n	$1838.685239091107 m_e$
Unified atomic mass constant	m_u	$1822.888479031408 m_e$
Avogadro constant	N_a	$6.022141990 \times 10^{23} mol^{-1}$
Boltzmann constant	k	$3.16681520371153 \times 10^{-6} \hbar^2 K^{-1} a_0^{-2} m_e^{-1}$
Faraday constant	$Faraday$	$6.022141991747723 \times 10^{23} e mol^{-1}$
Molar gas constant	R_{gas}	$1.907101047994109 \times 10^{18} \hbar^2 K^{-1} mol^{-1} a_0^{-2} m_e^{-1}$
Fine structure constant	α	0.007297352522615556
Rydberg constant	R_∞	$0.0005807048641344865 a_0^{-1}$
Bohr Magneton	μ_B	$0.5 e \hbar m_e^{-1}$
Electron magnetic moment	μ_e	$0.5005801751848031 e \hbar m_e^{-1}$
Landé g-factor for		
the free electron	g_e	2.002320700739213
Nuclear magneton	μ_N	$0.0002723085122457884 e \hbar m_e^{-1}$
Proton magnetic moment	μ_p	$0.000760516627687762 e \hbar m_e^{-1}$
Proton magnetogiric ratio	γ_p	$0.001521031723472069 e m_e^{-1}$
Magnetic moment of		
protons in H_2O	μ'	$0.0007604965645 e \hbar m_e^{-1}$
Proton resonance frequency		
per field in H_2O	γ'	$0.001520992639504675 e m_e^{-1}$

Stefan-Boltzmann constant		$8.80988087157682 \times 10^{-28} \hbar^3 K^{-4} a_0^{-6} m_e^{-2}$
Magnetic flux quantum	ϕ_0	$3.141592652725856 \hbar e^{-1}$
Conductance quantum		$0.3183098866547112 e^2 \hbar^{-1}$
Planck mass		$2.38945532716683 \times 10^{22} m_e$
Planck length		$3.05398157366997 \times 10^{-25} a_0$
Planck time		$2.228598019457374 \times 10^{-27} a_0^2 m_e \hbar^{-1}$
Electron Volt	eV	$0.03674932587122423 \hbar^2 a_0^{-2} m_e^{-1}$
First radiation constant		$741359.8822745807 \hbar^3 a_0^{-2} m_e^{-2}$
Second radiation constant		$2.718891138368016 \times 10^8 K a_0$
Quantum of circulation		$3.141592653589793 \hbar m_e^{-1}$

Table 9.3: A list of the conversion factors from SI and cgs to atomic units.

meter	m	$1.889726133921252 \times 10^{10} a_0$
Ångström	\AA	$1.889726133921252 a_0$
micron	μ	$18897.26133921252 a_0$
x unit	X	$0.001893505586189094 a_0$
fermi	F	$0.00001889726133921252 a_0$
barn	b	$3.57106486122496 \times 10^{-8} a_0^2$
litre	l	$6.748334594184675 \times 10^{27} a_0^3$

second	<u>s</u>	<u>$4.134137337414122 \times 10^{16} a_0^2 m_e \hbar^{-1}$</u>
minute	<u>min</u>	<u>$2.480482402448473 \times 10^{18} a_0^2 m_e \hbar^{-1}$</u>
hour	<u>h</u>	<u>$1.488289441469084 \times 10^{20} a_0^2 m_e \hbar^{-1}$</u>
gram	<u>g</u>	<u>$1.097769325266227 \times 10^{27} m_e$</u>
Unified Atomic Mass	<u>u</u>	<u>$1822.888479031408 m_e$</u>
Dalton	<u>Da</u>	<u>$1822.888479031408 m_e$</u>
coulomb	<u>C</u>	<u>$6.241509744511525 \times 10^{18} e$</u>
franklin	<u>Fr</u>	<u>$2.081942956418242 \times 10^9 e$</u>
abcoulomb		<u>$6.241509744511525 \times 10^{19} e$</u>
Charge density	<u>Cm^{-3}</u>	<u>$9.24896306992557 \times 10^{-13} e a_0^{-3}$</u>
Charge density (ESU)	<u>$Fr cm^{-3}$</u>	<u>$3.085121117456655 \times 10^{-16} e a_0^{-3}$</u>
Velocity	<u>ms^{-1}</u>	<u>$4.571028922573879 \times 10^{-7} \hbar a_0^{-1} m_e^{-1}$</u>
Acceleration	<u>ms^{-2}</u>	<u>$1.105679020676423 \times 10^{-23} \hbar^2 a_0^{-3} m_e^{-2}$</u>
Momentum	<u>$kgms^{-1}$</u>	<u>$5.017935336106338 \times 10^{23} \hbar a_0^{-1}$</u>
Hertz	<u>Hz</u>	<u>$2.418884324306202 \times 10^{-17} \hbar a_0^{-2} m_e^{-1}$</u>
Newton	<u>N</u>	<u>$1.21378051248898 \times 10^7 \hbar^2 a_0^{-3} m_e^{-1}$</u>
Pascal	<u>Pa</u>	<u>$3.398931578276133 \times 10^{-14} \hbar^2 a_0^{-5} m_e^{-1}$</u>
bar	<u>bar</u>	<u>$3.398931578276133 \times 10^{-9} \hbar^2 a_0^{-5} m_e^{-1}$</u>

Joule	<u>J</u>	<u>$2.293712755294755 \times 10^{17} \hbar^2 a_0^{-2} m_e^{-1}$</u>
erg	<u>erg</u>	<u>$2.293712755294755 \times 10^{10} \hbar^2 a_0^{-2} m_e^{-1}$</u>
rydberg	<u>Ry</u>	<u>$0.5 \hbar^2 a_0^{-2} m_e^{-1}$</u>
electronvolt	<u>eV</u>	<u>$0.03674932587122423 \hbar^2 a_0^{-2} m_e^{-1}$</u>
calorie, thermochemical	<u>cal_{th}</u>	<u>$9.59689416815326 \times 10^{17} \hbar^2 a_0^{-2} m_e^{-1}$</u>
Power, P	<u>W</u>	<u>$5.548225828243671 \hbar^3 a_0^{-4} m_e^{-2}$</u>
Action, L, J	<u>Js</u>	<u>$9.48252354296707 \times 10^{33} \hbar$</u>
Action (ESU)	<u>erg s</u>	<u>$9.48252354296707 \times 10^{26} \hbar$</u>
Thermodynamic Temperature	<u>K</u>	<u>K</u>
Entropy, S	<u>JK⁻¹</u>	<u>$2.293712755294755 \times 10^{17} \hbar^2 K^{-1} a_0^{-2} m_e^{-1}$</u>
Molar Entropy, <u>S_m</u>	<u>S_m</u>	<u>$2.293712755294755 \times 10^{17} \hbar^2 K^{-1} mol^{-1} a_0^{-2} m_e^{-1}$</u>
Entropy unit	<u>e.u.</u>	<u>$9.59689416815326 \times 10^{17} \hbar^2 K^{-1} mol^{-1} a_0^{-2} m_e^{-1}$</u>
radian	<u>rad</u>	<u>rad</u>
degree	<u>deg</u>	<u>$0.0174532925199433 rad$</u>
minute	<u>'</u>	<u>$0.0002908882086657216 rad$</u>
second	<u>"</u>	<u>$4.84813681109536 \times 10^{-6} rad$</u>
Circular frequency	<u>rad s⁻¹</u>	<u>$2.418884324306202 \times 10^{-17} rad \hbar a_0^{-2} m_e^{-1}$</u>
Ampere	<u>A</u>	<u>$150.9749008100334 e \hbar a_0^{-2} m_e^{-1}$</u>

Current (ESU)		$5.035980618632953 \times 10^{-8} e \hbar a_0^{-2} m_e^{-1}$
Current (EMU)=biot	$ Bi $	$1509.749008100334 e \hbar a_0^{-2} m_e^{-1}$
volt	$ V $	$0.03674932587122423 \hbar^2 e^{-1} a_0^{-2} m_e^{-1}$
Electric Potential (ESU)	$ erg Fr^{-1} $	$11.01717387704435 \hbar^2 e^{-1} a_0^{-2} m_e^{-1}$
Ohm	$ \Omega $	$0.000243413479154821 \hbar e^{-2}$
Electric Field	$ Vm^{-1} $	$1.944690567144141 \times 10^{-12} \hbar^2 e^{-1} a_0^{-3} m_e^{-1}$
Electric Field (ESU)	$ Frcm^{-2}(4\pi\epsilon_0)^{-1} $	$5.830034001970176 \times 10^{-8} \hbar^2 e^{-1} a_0^{-3} m_e^{-1}$
Electric Field Gradient	$ Vm^{-2} $	$1.02908592532868 \times 10^{-22} \hbar^2 e^{-1} a_0^{-4} m_e^{-1}$
Electric Field		
Gradient (ESU)	$ Frcm^{-3}(4\pi\epsilon_0)^{-1} $	$3.085121117456655 \times 10^{-16} \hbar^2 e^{-1} a_0^{-4} m_e^{-1}$
Electric Dipole Moment	$ Cm $	$1.179474407932758 \times 10^{29} ea_0$
Electric Dipole		
Moment (ESU)	$ Frcm $	$3.934302014076826 \times 10^{17} ea_0$
debye	$ D $	$0.3934302014076827 ea_0$
Electric Quadrupole		
Moment	$ Cm^2 $	$2.228883612961829 \times 10^{39} ea_0^2$
Electric Quadrupole		
Moment (ESU)	$ Frcm^2 $	$7.434753334739994 \times 10^{25} ea_0^2$
Electric Dipole Polarizability	$ J^{-1}C^2m^2 $	$6.065100679049756 \times 10^{40} e^2 a_0^4 m_e \hbar^{-2}$
Electric Dipole		

Polarizability (ESU)	$(4\pi\epsilon_0)cm^3$	$6.748334594184674 \times 10^{24} e^2 a_0^4 m_e \hbar^{-2}$
First Electric Dipole		
Hyperpolarizability	$ J^{-2}C^3m^3$	$3.118799865397922 \times 10^{52} e^3 a_0^7 m_e^2 \hbar^{-4}$
First Electric Dipole		
Hyperpolarizability (ESU)	$ erg^{-2}Fr^3cm^3$	$1.157510731627746 \times 10^{32} e^3 a_0^7 m_e^2 \hbar^{-4}$
Second Electric Dipole		
Hyperpolarizability	$ J^{-3}C^4m^4$	$1.603751217849538 \times 10^{64} e^4 a_0^{10} m_e^3 \hbar^{-6}$
Second Electric Dipole		
Hyperpolarizability (ESU)	$ erg^{-3}Fr^4cm^4$	$1.985425939776565 \times 10^{39} e^4 a_0^{10} m_e^3 \hbar^{-6}$
Electric Displacement	$ Cm^{-2}$	$0.01747800722491089 ea_0^{-2}$
siemens	$ S$	$4108.235926260923 e^2 \hbar^{-1}$
farad	$ F$	$1.698401153366137 \times 10^{20} e^2 a_0^2 m_e \hbar^{-2}$
tesla	$ T$	$4.254382547308656 \times 10^{-6} \hbar e^{-1} a_0^{-2}$
gauss	$ G$	$4.254382547308656 \times 10^{-10} \hbar e^{-1} a_0^{-2}$
weber	$ Wb$	$1.519267602090268 \times 10^{15} \hbar e^{-1}$
maxwell	$ Mx$	$1.191348438809734 \times 10^{-26} \hbar ea_0^{-4}$
henry	$ H$	$1.00630475260382 \times 10^{13} a_0^2 m_e e^{-2}$
Magnetic Field	$ Am^{-1}$	$7.989247653402288 \times 10^{-9} e \hbar a_0^{-3} m_e^{-1}$
oersted	$ Oe$	$7.989247653402288 \times 10^{-6} e \hbar a_0^{-3} m_e^{-1}$

Magnetic Dipole Moment	JT^{-1}	$5.391411632096341 \times 10^{22} e\hbar m_e^{-1}$
Magnetic Dipole		
Moment (EMU)	$erg\ G^{-1}$	$5.39141163209634 \times 10^{19} e\hbar m_e^{-1}$
Magnetizability	JT^{-2}	$1.267260659365711 \times 10^{28} e^2 a_0^2 m_e^{-1}$

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