1.1 **Basic Physical Units**

1.1.1 SI Units

Basic Physical Data			
supplementary SI units.			
it	Abbreviation		
damental Units			
le	mol		
pere	A		
ter	m		
ıdela	cd		
ogram	kg		
ian	rad		
radian	sr		
vin	К		
ond	S		
ted derived units			
ad	F		
pere per square meter	A/m ²		
ılomb	С		
t	V		
m	Ω		
le	J		
tz	Hz		
wton	Ν		
nry	Н		
ber	Wb		
la	Т		
tt	W		
	supplementary SI units. it damental Units le pere ter ter tedela ogram ian radian vin ond ted derived units ad pere per square meter ilomb t m le tz vton nry ber la tt	Asupplementary SI units.itAbbreviationdamental UnitslemolpereAtermolpereAtermolgramkgianradradiansrvinKondsted derived unitsadFpere per square meterA/m²hombCtVmΩleJttzHzvtonNmyHberWblaTttW	

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1

Prefix	Symbol	Factor	Prefix	Symbol	Factor
yotta zetta exa peta tera giga	Y Z E P T G	$10^{24} \\ 10^{21} \\ 10^{18} \\ 10^{15} \\ 10^{12} \\ 10^{9} \\ 10^{6}$	deci centi milli micro nano pico	d c m μ n p	$ \begin{array}{c} 10^{-1} \\ 10^{-2} \\ 10^{-3} \\ 10^{-6} \\ 10^{-9} \\ 10^{-12} \\ 10^{-15} \end{array} $
mega kilo hecto deca	M k h da	10^{3} 10^{3} 10^{2} 10^{1}	femto atto zepto yocto	f a z y	10^{-13} 10^{-18} 10^{-21} 10^{-24}

 Table 1.2
 Standard prefixes for SI units.

1.1.2 cgs-Gaussian Units

For a useful overview of non-SI units, see [1].

 Table 1.3
 Comparison of SI and cgs units.

Quantity	Unit	Abbrev.	SI equivalent
Length	centimeter	cm	10 ⁻² m
Mass	gramme	g	10^{-3}kg
Time	second	s	1 s
Force	dyne	dyn	10^{-5} N
Energy	erg	erg	10 ⁻⁷ J
Power	erg per second	${\rm ergs^{-1}}$	$10^{-7} W$
Electrical charge	statcoulomb	statcoul	$(3 \times 10^9)^{-1} \mathrm{C}$
Current	statampere	statamp	$(3 \times 10^9)^{-1}$ A
Electric potential	statvolt	statvolt	300 V
Magnetic flux density	gauss	G	$10^{-4}{ m T}$

1.2

Maxwell's Electromagnetic Equations

Table 1.4 Maxwell's equations.

	SI	cgs-Gaussian	
$\nabla \times E$	$=-\frac{\partial B}{\partial t}$	$=-\frac{1}{c}\frac{\partial B}{\partial t}$	Faraday's law
$\nabla imes H$	$= \frac{\partial D}{\partial t} + J$	$= \frac{1}{c} \frac{\partial D}{\partial t} + \frac{4\pi}{c} J$	Ampere's law

Table 1.4 (continued)

	SI	cgs-Gaussian	
$\nabla \cdot D$	$= \rho_{c}$	$=4\pi\rho_{\rm c}$	Poisson equation
$\nabla \cdot B$	= 0 $= \epsilon_r \epsilon_0 E$	= 0 $= \epsilon_r E$	
B	$= \mu_{\rm r} \mu_0 H$	$= \mu_r H$	

Boundary conditions The boundary conditions at an interface for Maxwell's electromagnetic equations are that the tangential component of E, and the normal component of B, must each be continuous, where normal means parallel to the local normal vector to the interface, and tangential means in the plane perpendicular to the local normal.

1.3 Special Relativity

Assume standard inertial frames *S* and *S'*, with respective Cartesian coordinates (x, y, z), (x', y', z') aligned such that the origins *O*, *O'* are coincident at time t = t' = 0, with *S'* moving with velocity v with respect to *S*. Subscript \parallel will denote the direction of this mutual motion, and subscript \perp denotes the orthogonal plane. The Lorentz transformations of various physically significant quantities are given in the following table [2]:

Quantity	Transformation
Space-time	$\mathbf{r} = \gamma_{\mathrm{v}} \left(\mathbf{r}_{ }' + \mathbf{v} t' \right) + \mathbf{r}_{\perp}'$
	$t = \gamma_{\rm v} \left(t + v r_{\rm II}'/c^2 \right)$
Invariant	$r^2 - c^2 t^2$
Velocity	$\boldsymbol{u} = \left(\boldsymbol{u}_{\parallel}' + \boldsymbol{v} + \boldsymbol{u}_{\perp}'/\gamma_{\mathrm{v}}\right) / \left(1 + \boldsymbol{u}_{\parallel}' \boldsymbol{v}/c^{2}\right)$
Momentum-mass	$p = \gamma_{\rm v} \left(p'_{\parallel} + m' v \right) + p'_{\perp}$
	$mc = \gamma_{\rm v} \left(m'c + v p'_{\parallel} / c \right)$
Invariant	$p^2 - m^2 c^2$
Current and charge densities	$J = \gamma_{\mathrm{v}} \left(J_{\parallel}' + \nu \rho_{\mathrm{c}} ight) + J_{\perp}'$
	$\rho_{\rm c} = \gamma_{\rm v} \left(\rho_{\rm c}' + \nu J_{\parallel}'/c^2 \right)$
Invariant	$J^2 - c^2 \rho_{\rm c}^2$
Electric and magnetic fields	$E = E'_{\parallel} + \gamma_{\rm v} \left(E_{\perp} - \nu \times B' \right)$
	$B = B_{\parallel}^{\nu} + \gamma_{\rm v} \left(B_{\perp}^{\prime} + \nu \times E^{\prime} / c^2 \right)$

Table 1.5 Lorentz transformations.

1.4

Physical Constants

The values of the constants quoted here are the 2006 CODATA recommended values [3].

Quantity	Symbol	Value	Units
Speed of light in vacuum	С	299 792 458	${ m ms^{-1}}$
Magnetic constant	μ_0	$4\pi \times 10^{-7}$	${\rm Hm^{-1}}$
Electric constant	ϵ_0	$8.854187817\ldots imes 10^{-12}$	$\mathrm{F}\mathrm{m}^{-1}$
Vacuum impedance	Z_0	376.730 313 461	Ω
Gravitational constant	G	$6.67428(67) imes 10^{-11}$	${ m m^{3}kg^{-1}s^{-2}}$
Planck constant	h	$6.62606896(33) imes 10^{-34}$	Js
Planck mass	$m_{\mathcal{P}}$	$2.17644(11) \times 10^{-8}$	kg
Planck length	$l_{\mathcal{P}}$	$1.616252(81) \times 10^{-35}$	m
Planck time	$t_{\mathcal{P}}$	$5.39124(27) imes 10^{-44}$	s
Avogadro constant	$N_{\rm A}$	$6.02214179(30) \times 10^{23}$	mol^{-1}
Bohr magneton	$\mu_{\rm B}$	$927.400915(23) \times 10^{-26}$	$J T^{-1}$
Bohr radius	a_0	$0.52917720859(36) imes 10^{-10}$	m
Boltzmann constant	$k_{\rm B}$	$1.3806504(24) \times 10^{-23}$	J K ⁻¹
Elementary charge	е	$1.602176487(40) imes 10^{-19}$	С
Fine structure constant	α	$7.2973525376(50) \times 10^{-3}$	
	α^{-1}	137.035 999 679(94)	
Molar gas constant	R	8.314 472(15)	$J \text{ mol}^{-1} \text{ K}^{-1}$
Nuclear magneton	$\mu_{ m N}$	$5.05078324(13) imes 10^{-27}$	J^{-1}
Rydberg constant	R_{∞}	10 973 731.568 527(73)	m^{-1}
Stefan–Boltzmann constant	σ	$5.670400(40) imes 10^{-8}$	$\mathrm{Wm^{-2}K^{-4}}$
Thomson cross section	$\sigma_{\rm e}$	$0.6652458558(27) \times 10^{-28}$	m ²
Wien constant	Ь	$2.8977685(51) \times 10^{-3}$	тK
α Particle:			
Mass	m_{α}	$6.64465620(33) imes 10^{-27}$	kg
– electron mass ratio	$m_{\alpha}/m_{\rm e}$	$7.2942995365(31) imes 10^3$	
– proton mass ratio	$m_{\alpha}/m_{\rm p}$	3.972 599 689 51(41)	
Deuteron:			
Mass	md	$3.34358320(17) \times 10^{-27}$	kg
– electron mass ratio	$m_{\rm d}/m_{\rm e}$	$3.6704829654(16) \times 10^3$	
– proton mass ratio	$m_{\rm d}/m_{\rm p}$	1.999 007 501 08(22)	
magnetic moment	$\mu_{\rm d}$	$4.33073465(11) \times 10^{-27}$	J T ⁻¹

 Table 1.6
 Values of physical constants.

Quantity	Symbol	Value	Units
Electron:			
Mass	m _e	$9.10938215(45) imes 10^{-31}$	kg
– α particle mass ratio	$m_{\rm e}/m_{lpha}$	$1.3709335611(29) imes 10^{-4}$	
– proton mass ratio	$m_{\rm e}/m_{\rm p}$	$5.4461702177(24) imes10^{-4}$	
– deuteron mass ratio	$m_{\rm e}/m_{\rm d}$	$2.7244371170(58) imes 10^{-4}$	
– neutron mass ratio	$m_{\rm e}/m_{\rm d}$	$5.4386734459(33) imes10^{-4}$	
Magnetic moment	μ_{e}	$-928.476377(23) \times 10^{-26}$	$\rm JT^{-1}$
Charge to mass ratio	$-e/m_{\rm e}$	$-1.758820150(44) imes 10^{11}$	$\rm Ckg^{-1}$
Classical radius	r _e	$2.8179402894(58) imes 10^{-15}$	m
Helion (³ He nucleus):			
Mass	$m_{ m h}$	$5.00641192(25) imes 10^{-27}$	kg
– electron mass ratio	$m_{\rm h}/m_{\rm e}$	$5.4958852765(52) imes 10^3$	
– proton mass ratio	$m_{\rm h}/m_{\rm p}$	2.993 152 671 3(26)	
Neutron:			
Mass	m _n	$1.674927211(84) imes 10^{-27}$	kg
 electron mass ratio 	$m_{\rm n}/m_{\rm e}$	$1.8386836605(11) imes 10^3$	
– proton mass ratio	$m_{\rm n}/m_{\rm p}$	1.001 378 419 18(46)	
Magnetic moment	$\mu_{\rm n}$	$-0.96623641(23) imes 10^{-26}$	$\rm JT^{-1}$
Proton:			
Mass	$m_{\rm p}$	$1.672621637(83) \times 10^{-27}$	kg
 electron mass ratio 	$m_{\rm p}/m_{\rm e}$	$1.83615267247(80) imes 10^3$	
– neutron mass ratio	$m_{\rm p}/m_{\rm n}$	0.998 623 478 24(46)	
Magnetic moment	$\mu_{\rm p}$	$1.410606662(37) \times 10^{-26}$	$\rm JT^{-1}$

Table 1.6 (continued)

1.5 Dimensional Analysis

 Table 1.7 Dimensions of common variables.

		SI	Quantity		cgs
C q ρ _c S σ _c	$\frac{q^2 t^2}{l^2 m}$ q $\frac{q}{l^3}$ $\frac{q^2 t}{l^2 m}$ $\frac{q^2 t}{l^3 m}$	F C $C m^{-3}$ S $S m^{-1}$	capacitance charge charge density conductance conductivity	$ l \\ \frac{l^{3/2} m^{1/2}}{t} \\ \frac{m^{1/2}}{l^{3/2} t} \\ \frac{l}{t} \\ \frac{1}{t} $	cm statcoul statcoul cm^{-3} $cm s^{-1}$ s^{-1}
I J D	$\frac{\frac{q}{t}}{\frac{q}{l^2 t}}$	A A m ^{-2} C m ^{-2}	current current density displacement	$\frac{\frac{l^{3/2} m^{1/2}}{t^2}}{\frac{m^{1/2}}{l^{1/2} t^2}}$ $\frac{m^{1/2}}{\frac{m^{1/2}}{l^{1/2} t}}$	statamp cm^{-2} statcoul cm^{-2}

Table 1.7	(continued)

		SI	Quantity		cgs
η_v E	$\frac{\frac{m}{lt}}{\frac{ml}{qt^2}}$	$kg m^{-1} s^{-1}$ V m ⁻¹	dynamic viscosity electric field	$\frac{\frac{m}{lt}}{\frac{m^{1/2}l^{1/2}}{t}}$	P statvolt cm ⁻¹
ϕ	$\frac{l^2 m}{qt^2}$	V	electric potential	$\frac{m^{1/2}}{l^{1/2}t}$	statvolt
Ε ε	$\frac{\frac{ml^2}{t^2}}{\frac{m}{lt^2}}$	J J m ⁻³	energy energy density	$\frac{ml^2}{t^2}$ $\frac{m}{lt^2}$	erg erg cm ⁻³
F	$\frac{lm}{t^2}$	Ν	force	$\frac{lm}{t^2}$	dyn
ν L	$\frac{1}{t}$	Hz m	frequency length	$\frac{1}{t}$	Hz cm
Φ	$\frac{l^2 m}{at}$	Wb	magnetic flux	$\frac{l^{3/2}m^{1/2}}{t}$	Mx
В	$\frac{m}{qt}$	Т	magnetic flux density	$\frac{m^{1/2}}{l^{1/2}t}$	G
Η	$\frac{q}{lt}$	$\mathrm{A}\mathrm{m}^{-1}$	magnetic intensity	$\frac{m^{1/2}}{l^{1/2}t}$	Oe
μ	$\frac{l^2 q}{t}$	$J T^{-1}$	magnetic moment	$\frac{l^{5/2}m^{1/2}}{t}$	Oe cm ³
т	т	kg	mass	т	gram
ρ	$\frac{m}{l^3}$	$\rm kgm^{-3}$	mass density	$\frac{m}{l^3}$	$\rm gm cm^{-3}$
Р	$\frac{l^2 m}{t^3}$	W	power	$\frac{l^2 m}{t^3}$	${\rm ergs^{-1}}$
р	$\frac{m}{lt^2}$	Р	pressure	$\frac{m}{lt^2}$	$\rm dyn cm^{-2}$
R	$\frac{l^2 m}{q^2 t}$	Ω	resistance	$\frac{t}{l}$	$\rm scm^{-1}$
η	$\frac{l^3 m}{q^2 t}$	Ω m	resistivity	t	S
κ	$\frac{lm}{t^3}$	$\rm Wm^{-1}K^{-1}$	thermal conductivity	$\frac{lm}{t^3}$	$\rm erg cm^{-1} s^{-1} K^{-1}$
μ_0	$\frac{lm}{q^2}$	${\rm Hm^{-1}}$	vacuum permeability		
ϵ_0	$\frac{q^2t^2}{l^3m}$	$\mathrm{F}\mathrm{m}^{-1}$	vacuum permittivity		
A	$\frac{lm}{qt}$	${\rm Wb}{\rm m}^{-1}$	vector potential	$\frac{l^{1/2}m^{1/2}}{t}$	G cm
и	$\frac{l}{t}$	${\rm ms^{-1}}$	velocity	$\frac{l}{t}$	${\rm cms^{-1}}$

1.6

Ionization Energies of Gas-Phase Atoms and Molecules

The energies of first ionization E_i for certain gas-phase molecules are given here, selected from [4]

 Table 1.8 Ionization energies of gas-phase atoms and molecules

Substance	Formula	E _i /eV
Acetylene Ammonia	C ₂ H ₂ NH ₃	11.400 10.070
Argon	Ar	15.75962

Substance	Formula	E _i /eV
Boron	В	8.298 03
Calcium	Ca	6.11316
Carbon dioxide	CO ₂	13.773
Carbon monoxide	CO	14.014
Chlorine	Cl	12.967 64
Chlorine	Cl ₂	11.480
Chlorosilane	ClH ₃ Si	11.4
Cyanide	CN	13.5984
Disodium	Na ₂	4.894
Ethylene	C_2H_4	10.5138
Fluorine (atomic)	Fl	17.422
Fluorine	Fl ₂	15.697
Formaldehyde	CH ₂ O	10.88
Formic acid	CH_2O_2	11.33
Helium	He	24.587 41
Hydrogen (atomic)	Н	13.598 44
Hydrogen	H ₂	15.425 93
Hydrogen chloride	HCl	12.749
Hydrogen sulfide	H_2S	10.457
Hydroxyl	HO	13.0170
Krypton	Kr	13.999 961
Mercury	Hg	10.437 50
Methane	CH_4	12.61
Methanol	CH ₃ OH	10.85
Methyl	CH ₃	9.843
Methylene	CH ₂	10.396
Neon	Ne	21.564 54
Nitrogen	Ν	14.534 14
Nitrogen	N ₂	15.5808
Oxygen	0	13.618 06
Oxygen	O ₂	12.0697
Silane	SiH_4	11.00
Silicon	Si	8.151 69
Sodium	Na	5.13908
Tetrachloromethane	CCl ₄	11.47
Tetrachlorosilane	SiCl ₄	11.79
Water	H ₂ O	12.6206
Xenon	Xe	12.12987

Table 1.8 (continued)

1.7

Electron Affinities of Selected Atoms and Molecules

The electron affinity E_A is defined to be the energy difference between the ground state of the neutral, and the lowest energy state of the corresponding negative ion. If $E_A > 0$, then the negative ion is stable; if $E_A < 0$, the negative ion is unstable. Selected data is presented below, drawn from [4, 5]

Substance	Formula	E _i /eV
Aluminum	Al	0.4328
Argon	Ar	-
Beryllium	Be	-
Boron	В	0.2797
Calcium	Ca	0.024 55
Carbon	С	1.262
Chlorine (atomic)	Cl	3.613
Chromium	Cr	0.675 84
Cobalt	Со	0.663 3
Copper	Cu	1.235
Deuterium	D	0.745 6
Fluorine (atomic)	F	3.401
Helium	He	-
Hydrogen	Н	0.7541
Iron	Fe	0.151
Krypton	Kr	-
Lithium	Li	0.6180
Magnesium	Mg	-
Manganese	Mn	-
Nickel	Ni	1.157 16
Nitrogen (atomic)	Ν	-
Neon	Ne	-
Oxygen (atomic)	0	1.461
Phosphorus	Р	0.7465
Potassium	Κ	0.501 459
Scandium	Sc	0.188
Silicon	Si	1.390
Sodium	Na	0.547 9
Sulfur	S	2.077
Titanium	Ti	0.084
Tritium	Т	0.7548
Vanadium	V	0.525
Xenon	Xe	-

 Table 1.9 Electron affinities of selected atoms and molecules.

Substance	Formula	E _i /eV
Diatomic	molecules	
Carbon	C ₂	3.27
Chlorine	Cl ₂	2.28
Cyanide	CN	3.862
Fluorine	F ₂	3.01
Methylidine radical	CH	1.238
Oxygen	O ₂	0.450
Disilicon	Si ₂	2.201
	SiH	1.277
	TiO	1.30
Triatomic	molecules	
	C ₃	1.981
	CCl ₂	1.593
	CF ₂	0.180
	CH_2	0.652
	C ₂ O	2.311
Ozone	O ₃	2.103
	SiF ₂	0.10
	Si ₂ F	1.99
	SiH ₂	1.124
	Si_2H	2.31
	Si ₃	2.29
Titanium dioxide	TiO ₂	1.59
Water	H ₂ O	1.078

Table 1.9 (continued)

1.8 Atomic and Molecular Notation

1.8.1 Atomic Electron Configurations

The electronic configuration in atoms is characterized by four quantum numbers (n, l, m_1, m_s) that define the distribution of electrons across the available atomic levels and orbitals, with no two electrons allowed to share the same four quantum numbers (the Pauli Principle). The classification is arranged in descending significance in terms of energy contribution.

1.8.1.1 Principal Quantum Number, n

Levels are denoted by the principal quantum number, n, which can take integer values n = 1, 2, 3... and which is the main determinant of electron energy. Atomic states with different n have significantly different energies. Historical notation for the principal quantum number is K(n = 1), L(n = 2), M(n = 3) and so on, alphabetically (a notation usually used in X-ray spectra). For each value of n, there are n subshells, identified by the angular momentum (or azimuthal) quantum number l.

1.8.1.2 Azimuthal Quantum Number, I

Each subshell or sublevel (sometimes referred to as orbital) is denoted by the angular momentum (or azimuthal) quantum number l, which can take take integer values from 0 to n-1. These refer to the quantization of the orbital angular momentum of an electron in the subshell, and leads to the overall shape of the orbital (see Figure 1.1). A conventional notation for the first four l-values is s(l = 0), p(l = 1), d(l = 2) and f(l = 3); the notation continues alphabetically with g(l = 5) and so on. Each subshell can contain a maximum of 2(2l + 1) electrons, which can occupy states characterized by m_l and m_s .



Figure 1.1 The angular dependence of the s, p and d orbitals, showing symmetry about the principal (horizontal) axis.

1.8.1.3 Magnetic Quantum Number, m1

Given that an electron is in subshell l, its angular momentum component along the principal axis (the main symmetry axis for the wavefunctions) is further quantized by the magnetic quantum number m_l , which can take integer values in the range (-l, -l + 1, ..., 0, ..., l - 1, l), yielding 2l + 1 states in total.

1.8.1.4 Spin Quantum Number, m_s

Finally, there are two spin states for each electron in any *n*, *l*, *m*_l state: spin-up and spin-down, corresponding to $m_s = \pm \frac{1}{2}$.

As a consequence of the distribution of electrons across the possible angular momentum, magnetic and spin quantum states, the total number of electrons in each of the principal quantum levels is $2n^2$, as can be seen from Table 1.10. In the standard notation for the configuration of electrons in an atom, each shell and subshell is given as a character string, with the number of electrons in each subshell stated as a superscript on the *l* value: for example, the configuration of electrons in He can be stated as $1s^2$; for Carbon atoms, $1s^22s^22p^2$, and so on. The ground-state configuration of selected atoms is given in Table 1.11.

Table 1.10	Atomic notation: unc	ler each principa	l quantum numbe	er, the subshel	ls are d	lenoted,
along with	the number of electro	ons per subshell.				

	<i>n</i> = 1	(К)	<i>n</i> = 2	(L)	<i>n</i> = 3	(M)	<i>n</i> = 4	(N)	<i>n</i> = 5	(0)
l = 0	1s	2	2s	2	3s	2	4s	2	5s	2
l = 1			2p	6	3p	6	4p	6	5p	6
l = 2			1		3d	10	4d	10	5d	10
l = 3							4f	14	5f	14
l = 4									5g	18
Total		2		8		18		32	U	50

 Table 1.11
 Electronic configuration of ground states for selected atoms.

Atom	Ground state	Comment
Н	1s	
He	$1s^2$	filled K shell
Li	$1s^22s$	filled K shell
Be	$1s^22s^2$	filled K shell
В	1s ² 2s ² 2p	filled K shell
С	$1s^{2}2s^{2}2p^{2}$	filled K shell
Ν	$1s^{2}2s^{2}2p^{3}$	filled K shell
0	$1s^{2}2s^{2}2p^{4}$	filled K shell
F	$1s^{2}2s^{2}2p^{5}$	filled K shell
Ne	$1s^{2}2s^{2}2p^{6}$	filled K, L shells
Na	[Ne]3s	filled K, L shells
Si	[Ne]3s ² 3p ²	filled K, L shells
Ar	[Ne]3s ² 3p ⁶	filled K, L, M shells

Table	1.12	Selected significant spectral lines	of atomic and s	ingly ionized	elements,	as observed
in air,	and	chosen for the greatest relative int	ensity; * denote	s Fraunhofer	lines.	

Element	Description	Transition	Lines/nm
Ar ArII CaII ClII Fe H H H He Na	prominent lines prominent visible H, K prominent visible prominent visible Lyman Series Balmer Series Paschen Series prominent visible D ₂ , D ₁	Iransition 4s-4p 4s-4p 4s-4p 4s-4p(1st 4), 3d-4p $4s^2-4s4p$ n = 2, 3, → 1 n = 3, 4, → 2 n = 4, 5, → 3 2p-4d, 2s-2p, 2p-3d 3s-3p	Lines/nm 696.54, 706.72 472.69, 4879.86 $393.36, 396.85^{*}$ 479.45, 489.68, 490.48, 521.80, 542.32 $385.992, 404.582, 438.356^{*}$ $121.5(\alpha), 102.5(\beta), 97.2(\gamma), 94.9(\delta) \dots 91.12$ $656.3(\alpha), 486.1(\beta), 434.1(\gamma), 410.2(\delta) \dots 634.6^{*}$ $1870, 1280, 1090, 1020, 954 \dots 820$ $447.15, 501.57, 587.56, 667.81^{*}$ $588.997, 589.594^{*}$ 615.60, 615.69, 615.82
OII	prominent visible		391.19, 397.32, 407.59, 441.49, 464.18, 464.91

Atomic spectra arise when electrons make the transition from one set of (n, l, m_1, m_s) to another, losing energy by emission of photons (or gaining energy by absorption). Examples of important spectra are given in Table 1.12.

1.8.1.5 Multielectron Atoms

For atoms with several electrons [6], there is strong electrostatic coupling between the orbital angular momentum and the spins across the populated states, leading to additional energy structure in the electronic configuration.

The total resultant orbital angular momentum vector arising from the l_i of the electrons in the atom is a quantum vector denoted as L. The underlying quantization comes from the interaction of electrons with different values of n and l, and is expressed in the quantum-mechanical vector addition of the associated vector angular momenta l_i to produce a resultant total orbital angular momentum L, the possible quantized values of which are given by m_l . In a similar way, the resultant of the quantum spins over the $m_{s,i}$ is designated by S. These resultants, L and S, can be added to produce a total resultant angular momentum J of the electrons in the atom, which is also quantized. The magnitude of the quantized resultant of L and S can only take the values L + S, L + S - 1, ..., |L - S|, denoted by J (this is a general rule for all quantum vectors).

The states L = 0, 1, 2, 3, ... are labeled *S*, *P*, *D*, *F* by analogy with the *l* values, with the series continuing alphabetically beyond L = 4. (Note that electrons in closed shells do not contribute to this coupling.) An additional fine-structure arises in each *L*-state, when magnetic interactions (from the intrinsic dipole moments of the electrons) are taken into account. States that are formed in this way are deemed to have multiplicity 2S + 1 and form multiplet states, designated by the *L* value letter, with left superscript showing the multiplicity of the state, and right subscript giving the corresponding *J* value.

For example, if an atom has an *f*-electron (l = 3) and a *d*-electron (l = 2), then the possible values of *L* are 3 + 2 = 5, 4, 3, 2 and |3 - 2| = 1. In a similar way, the possible values of *S* are 0 and 1. Hence, the multiplet states are *P*, *D*, *F*, *G* and *H*, each of which can have S = 0 (with multiplicity 1, and therefore are singlet states) or S = 1 (with multiplicity 3, and so are triplet states). The singlet states are then ${}^{1}P_{1}(L = 1, S = 0, J = 1)$, ${}^{1}D_{2}(L = 2, S = 0, J = 2)$ and so on, with the triplet states as ${}^{3}P_{2}(L = 1, S = 1, J = 2)$, ${}^{3}D_{3}(L = 2, S = 1, J = 3)$ and so on.

1.8.1.6 Selection Rules for Transitions

For electric dipole transitions, the following rules apply:

- 1. Δn unrestricted
- 2. $\Delta l = \pm 1$
- 3. $\Delta L = 0, \pm 1 \text{ except } 0 \nleftrightarrow 0$
- 4. $\Delta S = 0$
- 5. $\Delta J = 0, \pm 1 \text{ except } 0 \nleftrightarrow 0$

1.8.1.7 Emission and Absorption

The spectral emission coefficient $\varepsilon(v)$ due to a spontaneous electronic transition from an upper state *u* to a lower state *l* in an atom resulting in the emission of a photon of frequency nu_0 is given by

$$\varepsilon = \frac{n_{\rm u}A_{\rm ul}}{4\pi}h\nu\Phi(\nu-\nu_0) \tag{1.1}$$

where n_u is the population of the upper level, A_{ul} is the Einstein coefficient for spontaneous emission, nu_0 is the line center defined by $hnu_0 = E_u - E_l$, where $E_{u,l}$ denotes the energy level of the upper and lower atomic states, and Φ is the line-shape function, which describes natural and instrumental line-broadening mechanisms.

In the case of electric dipole transitions, A_{ul} is defined to be

$$A_{\rm ul} = \frac{64\pi^4 \nu^3}{3\epsilon_0 h c^3} \mu_{\rm ul}^2 \tag{1.2}$$

where μ_{ul} is the transition dipole moment.

1.8.2

Molecular Electron Configurations

The configurations of electrons in molecules is more complicated than the single atom case because the nuclear motion of the constituent species influences the electron energy levels, along with the persistent internuclear electric field that bonds the molecule together [7, 8].

The ground electronic state of a molecule is designated by X, with excited states of the same multiplicity (i.e., spin quantum number in Section 1.8.2.3) as the

ground state denoted by *A*, *B*, *C*, . . . in ascending order of energy; if excited states have a different multiplicity from the ground state, then these states are labeled with lower-case letters *a*, *b*, *c*, . . . The details of the electronic configurations in such states is given in the following paragraphs, which apply mainly to diatomic molecules.

1.8.2.1 Born–Oppenheimer Approximation

The Born–Oppenheimer approximation separates out the nuclear motion (vibration and rotation) from the electron behavior, under the assumption that the electrons will move much faster than the heavier nuclei. This assumption means that the electronic transition energies E_{el} (a few eV) are taken to be much larger than the vibrational energies E_{vib} (around 0.1 eV), which in turn are much larger than the rotational energies E_{rot} (a few meV):

$$E_{\rm el} \gg E_{\rm vib} \gg E_{\rm rot}$$
 (1.3)

1.8.2.2 A Quantum Number

Assuming that the Born–Oppenheimer approximation (Section 1.8.2.1) holds, the electronic configuration is characterized in a similar way to atomic electrons in that the quantum numbers (n_1 , l_1 , n_2 , l_2 , ...) produce different quantized energy levels associated with the quantum vectors L, S and J; however, the quantizing axis is the internuclear one, and the resultant orbital angular momentum along this axis is designated Λ , with states $\Lambda = 0, 1, 2, ...$ given the notation Σ , Π , Δ and so on, analogous with the *S*, *P*, *D* atomic *L* states.

1.8.2.3 Spin Quantum Number

Coupling of electron spins to the internuclear axis is weak, and so the resultant (total) S is much the same as for atoms; however, S, the axial component of S (and not to be confused with the Greek letter indicating the Λ value), plays a key role in diatomic molecules, coupling to Λ to form a resultant Ω , the total electronic angular momentum along the internuclear axis. $\Omega = |\Lambda + S|$, in a similar way to J for atoms. Hence, Ω can take the values $\Lambda + S$, $\Lambda + S - 1$, ..., $|\Lambda - S|$, and such states are deemed to have a (spin) multiplicity 2S + 1 (known as spin-splitting). Each such state can be subdivided into two Λ -substates, giving a total degeneracy of $(2S + 1)(2 - \delta_{0,\Lambda})$ where $\delta_{i,j} = 1$ if i = j and 0 otherwise, is the Kronecker delta.

1.8.2.4 Molecular Term Notation

The molecular notation then is as follows: the Λ state is written with a left superscript denoting the associated multiplicity of the of Σ value, and a right subscript giving the maximum Ω value. Hence, a state with S = 0, $\Lambda = 0$ is written as ${}^{1}\Sigma$ (see Table 1.13); for the state with S = 1, $\Lambda = 1$ (and therefore, $\Omega = 2$) is written by ${}^{3}\Pi_{2}$. This notation is preceded by a letter denoting the multiplicity of the state: *X* is ground state, and multiplicities are given by *A*, *B*, *C* if they have the same multiplicity as the ground state, otherwise lower case letters are used.

Term	State		g
${}^{1}\Sigma$ ${}^{2}\Pi$ ${}^{3}\Sigma$ ${}^{3}\Pi$ ${}^{2}\Delta$	singlet sigma	$S = 0, \Lambda = 0$	1
	doublet pi	$S = 1/2, \Lambda = 1$	4
	triplet sigma	$S = 1, \Lambda = 0$	3
	triplet pi	$S = 1, \Lambda = 1$	6
	doublet delta	$S = 1/2, \Lambda = 3$	4

 Table 1.13
 Molecular electronic state notation, showing the associated quantum numbers and electron degeneracy g.

1.8.2.5 Symmetry

The symmetry of the electron orbitals is a further complication: for a homonuclear molecule, the electron density must be symmetric with respect to the midpoint between the nuclei (that is, the center of mass), but the wavefunction of the electron can be even or odd parity, denoted g or u, respectively (from the German *gerade* and *ungerade*). For Σ states, symmetry of the wavefunction with respect to a mirror reflection through a plane containing the internuclear axis is denoted by a right superscript + if symmetric; – if not.

1.8.2.6 Selection Rules for Transitions

Electric dipole transitions between electronic levels in diatomic molecules obey the following selection rules:

- 1. $\Delta \Sigma = 0$ (no change in total electron spin)
- 2. $\Delta \Lambda = 0, \pm 1$
- 3. $u \leftrightarrow g$
- 4. $\Sigma^+ \leftrightarrow \Sigma^+$ or $\Sigma^- \leftrightarrow \Sigma^-$

The spectra of molecules is considerably more complex than that of atoms because of the more extensive range of possible transitions. Molecular spectra consist of bands, which are very tightly grouped series of emission (or absorption) lines within an amplitude envelope that may extend only for a few nanometers. The spacing of the lines within the band head is controlled by electron transitions between the molecule's rotational states. The envelopes are not symmetric: the conspicuous sharp edge is termed the band head, with the envelope fading smoothly in amplitude towards increasing wavelength (termed 'degraded to red') or decreasing wavelength ('degraded to violet').

Certain molecules exhibit very extensive band systems that span wide spectral ranges with little variation in band intensity or structure, such as H₂ (more than 100 strong bands between 406 and 835 nm), Cl₂ (mixture of continuum and band emission in 480–600 nm, strong continuous absorption in 250–400 nm), CO (198–860 nm, including third positive, Asundi, triplet, Cameron, 3A, Knauss & Kaplan bands, in addition to those in Table 1.14).

Table 1.14 Selected significant molecular spectral bands, as observed in air, and chosen for greatest relative intensity; § denotes extensive number of bands of similar intensity in the indicated wavelength range, with more

prominent heads identified in final column; r, v denotes degraded to red, violet; * denotes forbidden line. Data taken from [9], with additional information on ozone from [10].

Mol.	System	Range/nm	Prominent bands/nm
C ₂	Swan system	436–668v	471.52 473.71 516.52 558.55 563.55
C ₂	high-pressure system	341–786v	468.02 589.93 644.23
C ₂	Spark system	339–410v	360.73 385.22 410.23
Cl_2	conts absorption 250–400 nm	480–>600r§	continua + bands
Cl_2^+		394–487r	454.91 461.36 468.26 475.10 479.47
CH	430 system ^{<i>a</i>}	430–489v	431.25 431.5 438.4
CH	390 system	387–403r	387.11 388.9
CH	314 system	314–316rv ^b	314.34 314.41 314.49 315.66
CH^+		374–480r	374.37 395.44 422.53 ^c
CH_2	comet head group	398-408	403.91 404.21 405.15
CN	cyanogen red	470–940r§	635.51 650.23 787.4 914.05 939.3
CN	cyanogen violet	358–460v	387.14 388.34 421.60
CO	Angstrom	412–662v	451.09 483.53 519.82 561.02
CO	Herzberg	368–571v	389.31 412.48 438.03
CO	fourth positive	201–279r§	204.63 206.76 208.99 219.68 222.15 246.32
CO^+	first negative	200–315r	218.98 229.96 244.58 247.42 250.46 257.77
CO^+	comet tail	308–640r	379.58 401.97 427.43 456.58
CO ₂	Duffenback & Barker	280–500r	313.29 324.69 337.00 350.32 366.16
CO ₂	288.3 & 289.6 narrow bands	287–289	288.18 288.40 289.75
H_2O	infrared absorption	572–955	816.45 817.70 822.70 900.02 934.40 944.09
H_2O	emission bands	568–967r	716.45 809.7 891.6 927.7 966.9
H_2O_2	continuous absorption	< 215-370	peak at 300
He ₂	complex structure of bands	320–640r	462.56 464.85 573.30v 639.87
N ₂	first positive	503–1042v§	580.43 646.85 654.48 891.16 1042
N_2	second positive	281–498v	337.13 357.69 375.54 380.49
NH	strong peak		336.0 337.0
NH_3	Schuster broad emission	500-600	563.5 567.0 maxima
NH_3	UV absorption	<230r	201.09 204.84 208.64 212.65 216.73
NO	β -system	201–527r∬	289.26 304.30 320.69 338.64 358.35 380.09
O ₂	Hopfield emission	203–222v	203.08 207.66 212.31 217.00 221.75
O ₂	atmospheric absorption	538–551r	686.72* 759.37*
O3	Hartley broad absorption band	200-310	broad continuum, max at 255
O ₃	Huggins absorption	310-360	uv continuum + peaks, max 308
O ₃	Chappuis absorption	375–650	continuum + vibrational bands, max 602.5
OH	306.4 nm emission	244–402r	302.12 306.36 306.72 307.8 308.9
OH	visible ^d	370–580r	512.35 548.03

^{*a*} Seen in emission in comet tails, but in absorption in solar spectrum.

^{*b*} 314.34 is only v, and is most intense.

^c Seen in absorption in stellar spectra.

^d Can be detected in sunspots.

1.9 Characteristic Parameters for Typical Plasmas

1.9.1 Laboratory Plasma Reactors

There is a wide variety of vessel and electrode geometry in laboratory devices; the following list is indicative, but not exhaustive. Table 1.16 gives typical operating parameters for various plasma devices.

1.9.1.1 Corona Discharge

Also known as 'point-to-plane' discharge [11, 12], the ionizing electric field is produced by a marked asymmetry in the electrodes. The standard configuration, shown in Figure 1.2, is a sharply pointed electrode paired with a planar electrode, with the former producing a localized high electric field sufficient to ionize the neutral gas, and strike a plasma; a similar effect can be produced by electrodes in the form a wire inside a hollow cylinder. The ionization region is generally confined to a small area close to the high-field electrode, producing a drift region (between the ionization region and the flat electrode) in which charged particles (mainly electrons) react with neutrals and induce electron-moderated chemical reactions, including radical production. If the electric field is very high, plasma streamers can extend the ionizing region to encompass the second electrode. It is suitable for use over a wide range of pressures (including atmospheric), with applications that include ozone production, surface modification and combustion promotion.

1.9.1.2 Dielectric Barrier Discharge

Also known as silent discharges, dielectric barrier discharges (DBD) [13] generally consist of a pair of AC-powered plane electrodes with at least one covered in a dielectric layer (Figure 1.3). The neutral gas breaks down in the usual manner, forming streamers. However, when the streamers bridge the gap between the elec-



Figure 1.2 Typical configuration of a point-to-plane corona discharge, showing a plasma ionization region close to the high field at the point electrode, and the region of ion drift impinging on the flat electrode plate.



Figure 1.3 Typical configuration of a dielectric barrier discharge (DBD), showing the powered electrodes and the dielectric layers; though two dielectric layers are shown, it is only necessary to have one dielectric layer present in the discharge gap.

trodes, the dielectric layer allows free charge to accumulate which significantly affects the ongoing development of the discharge, including self-quenching. In particular, charge accumulated from one half-cycle of AC power is available to enhance the field in the subsequent half-cycle.

1.9.1.3 GEC Reference Cell

A standard parallel plate, capacitively-coupled rf plasma reactor designed for researching plasma discharge phenomena of direct relevance to the plasma technology sectors [14]. By designing a standard reactor for general use in different plasma conditions, the effects of reactor geometry could be minimized. Figure 1.4 shows a simplified schematic of a typical arrangement; in fact, either electrode can be powered independently, and the electrode spacing can be adjusted. Not shown on the schematic are the 8 diagnostic ports in the midplane. The showerhead electrode has 169 equally spaced holes placed in concentric circles for smooth gas feeding; the reactor is designed to work at a base pressure close to 10^{-5} Pa. Gas flow rates in the range 2–25 sccm (standard cubic centimeters per second) can be accommodated. At 10 sccm, the reactor pressure is generally not below 8 Pa.

1.9.1.4 Hollow Cathode Discharge

Hollow cathode devices (HCDs) [15–17] have the cathode in the form of a cup or cylinder, closed at one end, with the anode near the open end of the cathode (Figure 1.5). This arrangement allows the HCD to operate in the transition between the glow-discharge and a low-pressure arc discharge, supporting high current density negative glow (electron current) enclosed within the cathode structure. Because of their greater efficiency compared to a conventional plane-parallel electrode arrangement, HCD are used in spectral analyses of gas samples, and are valuable as photon sources (lamps). Microhollow cathode discharges (MHCDs) are similar in concept to HCD but are very much smaller, having scale lengths in the 10 s of mm. MHCD are often referred to as microdischarges, though the latter term additionally refers to devices which are similar in topology to HCD, but operate at atmospheric pressures and using AC power.



Figure 1.4 Simplified schematic of a Gaseous Electronics Conference (GEC) Reference Cell, showing the showerhead upper electrode and powered lower.



Figure 1.5 Simplified schematic of a typical hollow cathode discharge arrangement.

1.9.1.5 Tokamak

The primary device for magnetic confinement fusion, the tokamak holds deuterium–tritium plasma in a toroidal chamber, shown schematically in Figure 1.6. The strong toroidal magnetic field (shown in bold arrow) is imposed by external field coils (not shown), and combines with the poloidal self-field of the plasma; the resultant helical magnetic field structure inhibits the plasma from touching the vacuum vessel. The toroidal (or major) radius *R* and poloidal (or minor) radius *r* are key



Figure 1.6 Schematic of a tokamak reactor, showing the major *R* and minor *r* radii for a circular cross-section vessel.

Tokamak	Major radius/m	Minor radius/m	Peak B (/ <i>T</i>)	Peak current/MA	Heating/MW
Alcator C-Mod	0.67	0.22	2	8	9.5
Asdex upgrade	1.65	0.5-0.8	3.1	1.6	27
COMPASS	0.56	0.23-0.38	2.1	0.4	1
DIII-D	1.66	0.67	2.2	3	31
ITER	6.2	2.0	5	15	110
JET	2.96	1.25-2.1	3.45	5	51
JT-60	3.4	1.0	4	3	55
KSTAR	1.8	0.5	3.5 ^{<i>a</i>}	2.0	28
MAST∬	1.5	-	0.84	2.0	7.5

 Table 1.15
 Selected critical data for various tokamaks. § denotes spherical tokamak.

^a Superconducting coils.

Table 1.16The operating parameters for rf parallel plate plasma etching, and high-density plasma reactor [18].

RF	High-Density
10^{-1} - 10^{3}	10 ⁻² -10
0.001-10	$10^{-4} - 10^{-1}$
50-10 ³	$10^{2}-5 \times 10^{3}$
0.1-100	0.1–20 or 2.45 GHz
$10-3 \times 10^{3}$	10-200
1–10	1–10
$10^{14} - 10^{17}$	$10^{16} - 10^{19}$
$10^{-7} - 10^{-4}$	$10^{-4} - 10^{-1}$
50-10 ³	10-500
$10^{-2}-5$	1-50
0	0-0.1
	RF $10^{-1}-10^{3}$ 0.001-10 $50-10^{3}$ 0.1-100 $10^{-3} \times 10^{3}$ 1-10 $10^{14}-10^{17}$ $10^{-7}-10^{-4}$ $50-10^{3}$ $10^{-2}-5$ 0

^a Standard cubic centimeters per second.

parameters in determining the reactor geometry. The main fusion reaction is as follows:

$${}_{1}^{2}D + {}_{1}^{3}T \rightarrow {}_{2}^{4}He + {}_{0}^{1}n$$
 (1.4)

where the neutron has 14.1 MeV energy. Deuterium is a naturally occurring isotope of hydrogen; tritium has a short half-life of 12.3 years, and so has negligible natural abundance. Instead, it can be bred from lithium via the following reactions:

$${}_{0}^{1}n + {}_{3}^{6}\text{Li} \rightarrow {}_{1}^{3}\text{T} + {}_{2}^{4}\text{He}$$
(1.5)

$${}_{0}^{1}n + {}_{3}^{7}Li \rightarrow {}_{1}^{3}T + {}_{2}^{4}He + {}_{0}^{1}n$$
(1.6)

Table 1.15 gives characteristic data for a range of tokamaks. Spherical tokamaks are devices in which the major radius is reduced to a minimum, as they are essen-

tially spheres with a central column dividing the chamber, making them formally toroidal in topological form.

1.9.2 Terrestrial and Solar Plasmas

The data in this section characterizes the distribution of neutral and ionized species throughout the atmospheres of the earth and the sun.

Ionospheric region	Height/km	$n_{\rm e}/{\rm m}^{-3}$ (day)	$n_{ m e}/{ m m}^{-3}$ (night)
D	50–90	10 ⁹	10 ⁸
E	90-140	10^{11}	$< 10^{10}$
F ₁	140-200	3×10^{11}	10^{10}
F ₂	200–400	10 ¹²	10 ¹¹

 Table 1.17
 Ionospheric parameters [19].

Tab	le 1	.18	Sola	r p	lasma	parameters	[20,	21]	
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Quantity	Region	Typical value
Total number density/m ⁻³	photosphere	10 ²² -10 ²³
Electron number density/ m^{-3}	photosphere	$10^{18} - 10^{20}$
Total number density/m $^{-3}$	chromosphere	$10^{16} - 10^{22}$
Electron number density/ m^{-3}	chromosphere	$10^{16} - 10^{18}$
Total number density/ m^{-3}	corona	$10^8 - 10^{15}$
Electron number density/m ⁻³	corona	$10^8 - 10^{15}$
Temperature/K	photosphere	4×10^{3} - 6×10^{3}
Temperature/K	chromosphere	$\sim 3\times 10^310^4$
Temperature/K	corona	> 10 ⁶
Magnetic field strength/T	poles	$\sim 10^{-4}$
Magnetic field strength/T	sunspot	~ 0.3
Magnetic field strength/T	prominence	$10^{-3} - 10^{-2}$
Magnetic field strength/T	chromospheric plage	$\sim 10^{-2}$



Figure 1.7 Model atmosphere MSIS E 90 from the Virtual Ionosphere, Thermosphere, Mesosphere Observatory (VITMO). The curves show the Nitrogen molecule number density (lefthand axis) and temperature (right-hand axis) as a function of height above sea level.



Figure 1.8 Model atmosphere as for Figure 1.7. The curves show the relative abundance by number of various chemical species (left-hand axis) and temperature (right-hand axis) as a function of height above sea level.





Plots shown are electron density (left-hand vertical axis), electron and ion temperatures (right-hand vertical axis) as functions of height.



Figure 1.10 Model Ionosphere based on International Reference Ionosphere IRI 2007, for which D region height is 88 km, E 110 km, F_2 350 km. Plots shown are electron density (left-hand vertical axis), and relative ion abundance (right-hand vertical axis) as functions of height.