1.3.4 Atoms and molecules

Name	Symbol	Definition	SI unit	Notes
nucleon number, mass number	A		1	
proton number, atomic number	Z		1	
neutron number	N	$N = A - Z$	1	
electron rest mass	m_e		kg	(1)
mass of atom, atomic mass	m_a, m		kg	
atomic mass constant	m_u	$m_u = m_a(^{12}C)/12$	kg	(1), (2)
mass excess	Δ	$\Delta = m_a - Am_u$	kg	
elementary charge, proton charage	e		C	
Planck constant	h		J s	
Planck constant/2π	$\hbar$	$\hbar = h/2\pi$	J s	
Bohr radius	a_0	$a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$	m	
Rydberg constant	R_∞	$R_\infty = E_h/2hc$	m^{-1}	
fine structure constant	α	$\alpha = e^2/4\pi\varepsilon_0\hbar c$ 1		
ionization energy	E_i		J	
electron affinity	E_{ea}		J	

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(1)   Analogous symbols are used for other particles with subscripts: p for proton, n for neutron, a for atom, N for nucleus, etc.

(2) m_u is equal to the unified atomic mass unit, with symbol u, i.e. $m_u = 1$ u. In biochemistry the name dalton, with symbol Da, is used for the unified atomic mass unit, although the name and symbols have not been accepted by CGPM.

Name	Symbol	Definition	SI unit	Notes
electronegativity	χ	$\chi = \frac{1}{2}(E_i + E_{ea})$ J		(3)
dissociation energy	E_d, D		J	
from the ground state	D_0		J	(4)
from the potential minimum	D_e		J	(4)
principal quantum number (H atom)	n	$E = -hcR/n^2$ 1		
angular momentum quantum numbers	see under Spectroscopy, section 3.5.			
magnetic dipole moment of a molecule	$\boldsymbol{m}, \boldsymbol{\mu}$	$E_p = -\boldsymbol{m} \cdot \boldsymbol{B}$ J T^{-1}		(5)
magnetizability of a molecule	ξ	$\boldsymbol{m} = \xi \boldsymbol{B}$	J T^{-2}	
Bohr magneton	μ_B	$\mu_B = eh/2m_e$	J T^{-1}	

(3)   The concept of electronegativity was intoduced by L. Pauling as the power of an atom in a molecule to attract electrons to itself. There are several ways of defining this quantity. The one given in the table has a clear physical meaning of energy and is due to R.S. Mulliken. The most frequently used scale, due to Pauling, is based on bond dissociation energies in eV and it is relative in the sense that the values are dimensionless and that only electronegativity differences are defined. For atoms A and B

$$\chi_{r,A} - \chi_{r,B} = (eV)^{-1/2} \sqrt{E_d(AB) - [E_d(AA) + E_d(BB)]}$$

where χ_r denotes the Pauling relative electronegativity. The scale is chosen so as to make the relative electronegativity of hydrogen $\chi_{r,H} = 2.1$. There is a difficulty in choosing the sign of the square root, which determines the sign of $\chi_{r,A}$ - $\chi_{r,B}$. Pauling made this choice intuitively.

(4)   The symbols D_0 and D_e are mainly used for diatomic dissociation energies.

(5)   Magnetic moments of specific particles may be denoted by subscripts, e.g. μ_e, μ_p, μ_n for an electron, a proton and a neutron.

Name	Symbol	Definition	SI unit	Notes
nuclear magneton	μ_N	$\mu_N = (m_e/m_p)\mu_B$	J T^{-1}	
magnetogyric ratio (gyromagnetic ratio)	γ	$\gamma = \mu/L$	s^{-1} T^{-1}	(6)
g-factor	g	$g = 2\mu/\mu_B$	1	
nuclear g-factor	g_N	$g_N = \mu/I\mu_N$	1	
Larmor angular frequency	ω_L	$\omega_L = (e/2m)B$	s^{-1}	(7)
Larmor frequency	ν_L	$\nu_L = \omega_L/2\pi$	Hz	
relaxation time,				
longitudinal	T_1		s	(8)
transverse	T_2		s	(8)
electric field gradient tensor	$\boldsymbol{q}$	$q_{\alpha\beta} = -\partial^2 V/\partial\alpha\partial\beta$	V m^{-2}	
activity (of a radioactive substance)	A	$A = -dN_B/dt$	Bq	(9)
decay (rate) constant, disintegration (rate) constant	λ, k	$A = \lambda N_B$	s^{-1}	(9)
half life	$t_{1/2}, T_{1/2}$	$N_B(t_{1/2}) = N_B(0)/2$	s	(9), (10)
mean life	τ	$\tau = 1/\lambda$	s	(10)
level width	Γ	$\Gamma = h/\tau$	J	
disintegration energy	Q		J	
cross section (of a nuclear reaction)	σ		m^2	

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(6) μ is the magnetic moment, L the angular momentum.

(7)   This quantity is commonly called Larmor circular frequency.

(8)   These quantities are used in the context of saturation effects in spectroscopy, particularly spin-resonance spectroscopy (see section 3.5).

(9) N_B is the number of radioactive atoms B.

(10)   Half lives and mean lives are often given in years (a), see conversion tables.
        $t_{1/2} = \tau \ln 2$ for exponential decays.