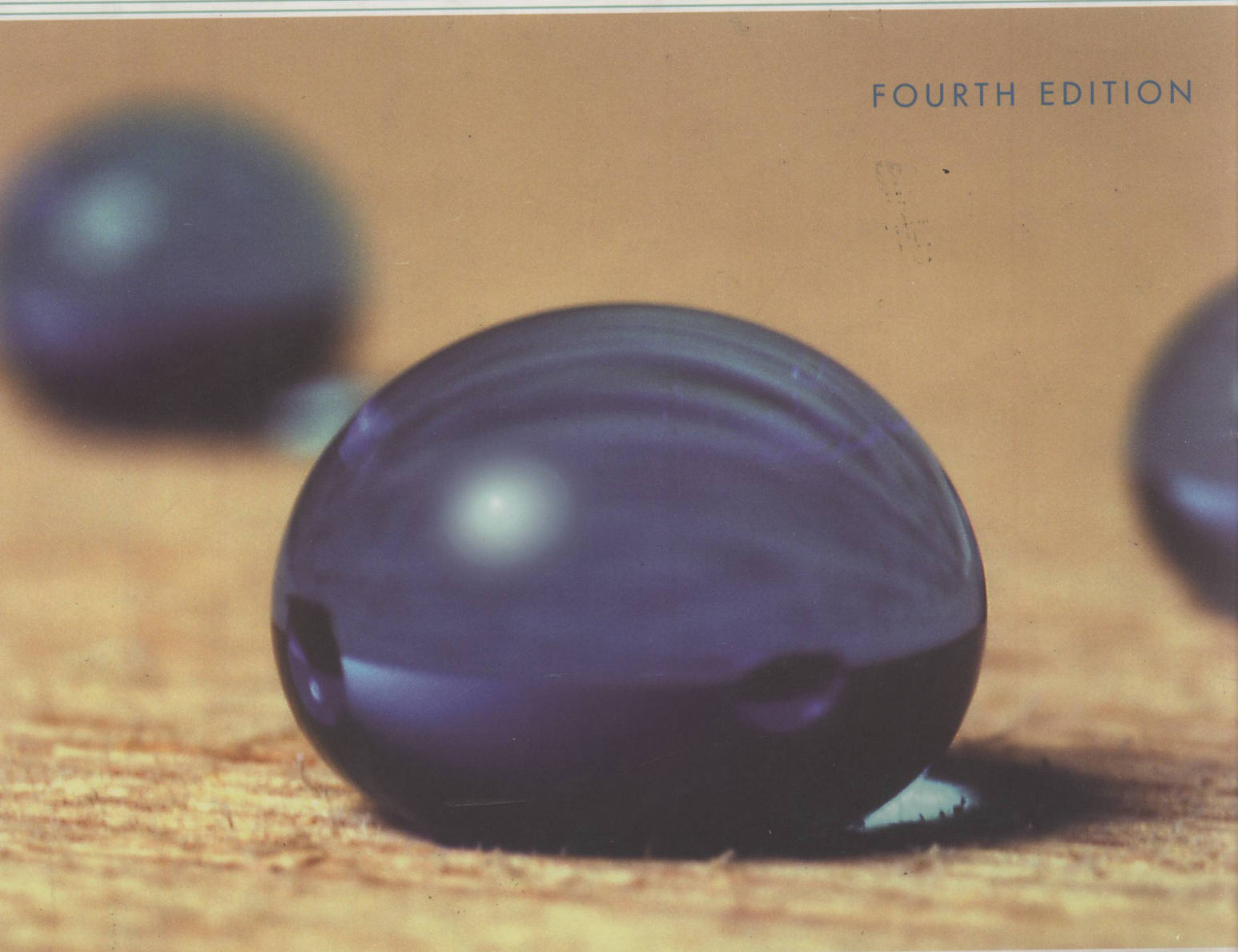


CHEMICAL PRINCIPLES

The Quest for Insight

FOURTH EDITION



PETER ATKINS / LORETTA JONES

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CONTENTS IN BRIEF

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The Quest for Insight

FOURTH EDITION

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University of Northern Colorado



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 IA IIA

PERIODIC TABLE OF THE ELEMENTS*

1			<div style="border: 1px solid black; padding: 5px; text-align: center;"> 1 H Hydrogen 1.0079 $1s^1$ </div>						
2	3 Li Lithium 6.94 $2s^1$	4 Be Beryllium 9.01 $2s^2$							
3	11 Na Sodium 22.99 $3s^1$	12 Mg Magnesium 24.31 $3s^2$	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII
4	19 K Potassium 39.10 $4s^1$	20 Ca Calcium 40.08 $4s^2$	21 Sc Scandium 44.96 $3d^1 4s^2$	22 Ti Titanium 47.87 $3d^2 4s^2$	23 V Vanadium 50.94 $3d^3 4s^2$	24 Cr Chromium 52.00 $3d^5 4s^1$	25 Mn Manganese 54.94 $3d^5 4s^2$	26 Fe Iron 55.84 $3d^6 4s^2$	27 Co Cobalt 58.93 $3d^7 4s^2$
5	37 Rb Rubidium 85.47 $5s^1$	38 Sr Strontium 87.62 $5s^2$	39 Y Yttrium 88.91 $4d^1 5s^2$	40 Zr Zirconium 91.22 $4d^2 5s^2$	41 Nb Niobium 92.91 $4d^4 5s^1$	42 Mo Molybdenum 95.94 $4d^5 5s^1$	43 Tc Technetium (98) $4d^5 5s^2$	44 Ru Ruthenium 101.07 $4d^7 5s^1$	45 Rh Rhodium 102.90 $4d^8 5s^1$
6	55 Cs Cesium 132.91 $6s^1$	56 Ba Barium 137.33 $6s^2$	71 Lu Lutetium 174.97 $5d^1 6s^2$	72 Hf Hafnium 178.49 $5d^2 6s^2$	73 Ta Tantalum 180.95 $5d^3 6s^2$	74 W Tungsten 183.84 $5d^4 6s^2$	75 Re Rhenium 186.21 $5d^5 6s^2$	76 Os Osmium 190.23 $5d^6 6s^2$	77 Ir Iridium 192.22 $5d^7 6s^2$
7	87 Fr Francium (223) $7s^1$	88 Ra Radium (226) $7s^2$	103 Lr Lawrencium (262) $6d^1 7s^2$	104 Rf Rutherfordium (261) $6d^2 7s^2$	105 Db Dubnium (262) $6d^3 7s^2$	106 Sg Seaborgium (266) $6d^4 7s^2$	107 Bh Bohrium (262) $6d^5 7s^2$	108 Hs Hassium (277) $6d^6 7s^2$	109 Mt Meitnerium (268) $6d^7 7s^2$

Lanthanoids 6
 (lanthanides)

57 La Lanthanum 138.91 $5d^1 6s^2$	58 Ce Cerium 140.12 $4f^1 5d^1 6s^2$	59 Pr Praseodymium 140.91 $4f^3 6s^2$	60 Nd Neodymium 144.24 $4f^4 6s^2$	61 Pm Promethium (145) $4f^5 6s^2$
89 Ac Actinium (227) $6d^1 7s^2$	90 Th Thorium 232.04 $6d^2 7s^2$	91 Pa Protactinium 231.04 $5f^2 6d^1 7s^2$	92 U Uranium 238.03 $5f^3 6d^1 7s^2$	93 Np Neptunium (237) $5f^4 6d^1 7s^2$

Actinoids 7
 (actinides)

*Molar masses (atomic weights) quoted to the number of significant figures given here can be regarded as typical of most naturally occurring samples.

13 14 15 16 17 18
 III IV V VI VII VIII
 IIIA IVA VA VIA VIIA VIIIA

2
 He
 Helium
 4.00
 $1s^2$

5 B Boron 10.81 $2s^2 2p^1$	6 C Carbon 12.01 $2s^2 2p^2$	7 N Nitrogen 14.01 $2s^2 2p^3$	8 O Oxygen 16.00 $2s^2 2p^4$	9 F Fluorine 19.00 $2s^2 2p^5$	10 Ne Neon 20.18 $2s^2 2p^6$
13 Al Aluminum 26.98 $3s^2 3p^1$	14 Si Silicon 28.09 $3s^2 3p^2$	15 P Phosphorus 30.97 $3s^2 3p^3$	16 S Sulfur 32.06 $3s^2 3p^4$	17 Cl Chlorine 35.45 $3s^2 3p^5$	18 Ar Argon 39.95 $3s^2 3p^6$

10 11 12
 IB IIB

28 Ni Nickel 58.69 $3d^8 4s^2$	29 Cu Copper 63.55 $3d^{10} 4s^1$	30 Zn Zinc 65.41 $3d^{10} 4s^2$	31 Ga Gallium 69.72 $4s^2 4p^1$	32 Ge Germanium 72.64 $4s^2 4p^2$	33 As Arsenic 74.92 $4s^2 4p^3$	34 Se Selenium 78.96 $4s^2 4p^4$	35 Br Bromine 79.90 $4s^2 4p^5$	36 Kr Krypton 83.80 $4s^2 4p^6$
46 Pd Palladium 106.42 $4d^{10}$	47 Ag Silver 107.87 $4d^{10} 5s^1$	48 Cd Cadmium 112.41 $4d^{10} 5s^2$	49 In Indium 114.82 $5s^2 5p^1$	50 Sn Tin 118.71 $5s^2 5p^2$	51 Sb Antimony 121.76 $5s^2 5p^3$	52 Te Tellurium 127.60 $5s^2 5p^4$	53 I Iodine 126.90 $5s^2 5p^5$	54 Xe Xenon 131.29 $5s^2 5p^6$
78 Pt Platinum 195.08 $5d^9 6s^1$	79 Au Gold 196.97 $5d^{10} 6s^1$	80 Hg Mercury 200.59 $5d^{10} 6s^2$	81 Tl Thallium 204.38 $6s^2 6p^1$	82 Pb Lead 207.2 $6s^2 6p^2$	83 Bi Bismuth 208.98 $6s^2 6p^3$	84 Po Polonium (209) $6s^2 6p^4$	85 At Astatine (210) $6s^2 6p^5$	86 Rn Radon (222) $6s^2 6p^6$
110 Ds Darmstadtium $6d^8 7s^2 (?)$	111 Rg Roentgenium $6d^{10} 7s^1 (?)$	112	113	114	115	116	117	118

Metals ← → Nonmetals
 Metalloids

62 Sm Samarium 150.36 $4f^6 6s^2$	63 Eu Europium 151.96 $4f^7 6s^2$	64 Gd Gadolinium 157.25 $4f^7 5d^1 6s^2$	65 Tb Terbium 158.93 $4f^9 6s^2$	66 Dy Dysprosium 162.50 $4f^{10} 6s^2$	67 Ho Holmium 164.93 $4f^{11} 6s^2$	68 Er Erbium 167.26 $4f^{12} 6s^2$	69 Tm Thulium 168.93 $4f^{13} 6s^2$	70 Yb Ytterbium 173.04 $4f^{14} 6s^2$
94 Pu Plutonium (244) $5f^6 7s^2$	95 Am Americium (243) $5f^7 7s^2$	96 Cm Curium (247) $5f^7 6d^1 7s^2$	97 Bk Berkelium (247) $5f^9 7s^2$	98 Cf Californium (251) $5f^{10} 7s^2$	99 Es Einsteinium (252) $5f^{11} 7s^2$	100 Fm Fermium (257) $5f^{12} 7s^2$	101 Md Mendelevium (258) $5f^{13} 7s^2$	102 No Nobelium (259) $5f^{14} 7s^2$

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CHEMICAL PRINCIPLES

THE ELEMENTS

Element	Symbol	Atomic number	Molar mass* (g·mol ⁻¹)	Element	Symbol	Atomic number	Molar mass* (g·mol ⁻¹)
Actinium	Ac	89	(227)	Mendelevium	Md	101	(258)
Aluminum	Al	13	26.98	Mercury	Hg	80	200.59
Americium	Am	95	(243)	Molybdenum	Mo	42	95.94
Antimony	Sb	51	121.76	Neodymium	Nd	60	144.24
Argon	Ar	18	39.95	Neon	Ne	10	20.18
Arsenic	As	33	74.92	Neptunium	Np	93	(237)
Astatine	At	85	(210)	Nickel	Ni	28	58.69
Barium	Ba	56	137.33	Niobium	Nb	41	92.91
Berkelium	Bk	97	(247)	Nitrogen	N	7	14.01
Beryllium	Be	4	9.01	Nobelium	No	102	(259)
Bismuth	Bi	83	208.98	Osmium	Os	76	190.23
Bohrium	Bh	107	(264)	Oxygen	O	8	16.00
Boron	B	5	10.81	Palladium	Pd	46	106.42
Bromine	Br	35	79.90	Phosphorus	P	15	30.97
Cadmium	Cd	48	112.41	Platinum	Pt	78	195.08
Calcium	Ca	20	40.08	Plutonium	Pu	94	(244)
Californium	Cf	98	(251)	Polonium	Po	84	(209)
Carbon	C	6	12.01	Potassium	K	19	39.10
Cerium	Ce	58	140.12	Praseodymium	Pr	59	140.91
Cesium	Cs	55	132.91	Promethium	Pm	61	(145)
Chlorine	Cl	17	35.45	Protactinium	Pa	91	231.04
Chromium	Cr	24	52.00	Radium	Ra	88	(226)
Cobalt	Co	27	58.93	Radon	Rn	86	(222)
Copper	Cu	29	63.55	Rhenium	Re	75	186.21
Curium	Cm	96	(247)	Rhodium	Rh	45	102.90
Darmstadtium	Ds	110	—	Roentgenium	Rg	111	—
Dubnium	Db	105	(262)	Rubidium	Rb	37	85.47
Dysprosium	Dy	66	162.50	Ruthenium	Ru	44	101.07
Einsteinium	Es	99	(252)	Rutherfordium	Rf	104	(261)
Erbium	Er	68	167.26	Samarium	Sm	62	150.36
Europium	Eu	63	151.96	Scandium	Sc	21	44.96
Fermium	Fm	100	(257)	Seaborgium	Sg	106	(266)
Fluorine	F	9	19.00	Selenium	Se	34	78.96
Francium	Fr	87	(223)	Silicon	Si	14	28.09
Gadolinium	Gd	64	157.25	Silver	Ag	47	107.87
Gallium	Ga	31	69.72	Sodium	Na	11	22.99
Germanium	Ge	32	72.64	Strontium	Sr	38	87.62
Gold	Au	79	196.97	Sulfur	S	16	32.06
Hafnium	Hf	72	178.49	Tantalum	Ta	73	180.95
Hassium	Hs	108	(277)	Technetium	Tc	43	(98)
Helium	He	2	4.00	Tellurium	Te	52	127.60
Holmium	Ho	67	164.93	Terbium	Tb	65	158.93
Hydrogen	H	1	1.0079	Thallium	Tl	81	204.38
Indium	In	49	114.82	Thorium	Th	90	232.04
Iodine	I	53	126.90	Thulium	Tm	69	168.93
Iridium	Ir	77	192.22	Tin	Sn	50	118.71
Iron	Fe	26	55.84	Titanium	Ti	22	47.87
Krypton	Kr	36	83.80	Tungsten	W	74	183.84
Lanthanum	La	57	138.91	Uranium	U	92	238.03
Lawrencium	Lr	103	(262)	Vanadium	V	23	50.94
Lead	Pb	82	207.2	Xenon	Xe	54	131.29
Lithium	Li	3	6.94	Ytterbium	Yb	70	173.04
Lutetium	Lu	71	174.97	Yttrium	Y	39	88.91
Magnesium	Mg	12	24.31	Zinc	Zn	30	65.41
Manganese	Mn	25	54.94	Zirconium	Zr	40	91.22
Meitnerium	Mt	109	(268)				

*Parentheses around molar mass indicate the most stable isotope of a radioactive element.

SI PREFIXES

z
zepto-
10^{-21}
a
atto-
10^{-18}
f
femto
10^{-15}
p
pico-
10^{-12}
n
nano-
10^{-9}
μ
micro-
10^{-6}
m
milli-
10^{-3}
c
centi-
10^{-2}
d
deci-
10^{-1}
da
deka-
10
h
hecto-
10^2
k
kilo-
10^3
M
mega-
10^6
G
giga-
10^9
T
tera-
10^{12}

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FUNDAMENTAL CONSTANTS

Name	Symbol	Value
Atomic mass constant	m_u	$1.660\ 54 \times 10^{-27}$ kg
Avogadro's constant	N_A	$6.022\ 14 \times 10^{23}$ mol ⁻¹
Boltzmann's constant	k	$1.380\ 66 \times 10^{-23}$ J·K ⁻¹
Fundamental charge	e	$1.602\ 18 \times 10^{-19}$ C
Faraday's constant	$F = N_A e$	$9.648\ 53 \times 10^4$ C·mol ⁻¹
Gas constant	$R = N_A k$	$8.314\ 47$ J·K ⁻¹ ·mol ⁻¹
		$8.314\ 47$ L·kPa·K ⁻¹ ·mol ⁻¹
		$8.205\ 74 \times 10^{-2}$ L·atm·K ⁻¹ ·mol ⁻¹
		$62.36\ 37$ L·Torr·K ⁻¹ ·mol ⁻¹
		$8.314\ 47 \times 10^{-2}$ L·bar·K ⁻¹ ·mol ⁻¹
Mass of electron	m_e	$9.109\ 38 \times 10^{-31}$ kg
Mass of neutron	m_n	$1.674\ 93 \times 10^{-27}$ kg
Mass of proton	m_p	$1.672\ 62 \times 10^{-27}$ kg
Planck's constant	h	$6.626\ 08 \times 10^{-34}$ J·s
	$\hbar = h/2\pi$	$1.054\ 57 \times 10^{-34}$ J·s
Rydberg constant	\mathcal{R}	$3.289\ 84 \times 10^{15}$ Hz
Speed of light	c	$2.997\ 92 \times 10^8$ m·s ⁻¹
Standard acceleration of free fall	g	$9.806\ 65$ m·s ⁻²
Vacuum permittivity	ϵ_0	$8.854\ 19 \times 10^{-12}$ J ⁻¹ ·C ² ·m ⁻¹

RELATIONS BETWEEN UNITS*

Property	Common unit	SI unit
Mass	2.205 lb (lb = pound)	1.000 kg
	1.000 lb	453.6 g
	1.000 oz (oz = ounce)	28.35 g
	1.000 ton (= 2000 lb)	907.2 kg
	1 t (t = tonne, metric ton)	10 ³ kg
Length	1.094 yd (yd = yard)	1.000 m
	0.3937 in. (in. = inch)	1.000 cm
	0.6214 mi (mi = mile)	1.000 km
	1 in.	2.54 cm
	1 ft (ft = foot)	30.48 cm
	1.000 yd	0.9144 m
	1 Å (Å = ångström)	10 ⁻¹⁰ m
Volume	1 L (L = liter)	10 ³ cm ³ , 1 dm ³
	1.000 gal (gal = gallon) [†]	3.785 dm ³ (3.785 L)
	1.00 ft ³ (ft ³ = cubic foot)	2.83 × 10 ⁻² m ³ (28.3 L)
	1.00 qt (qt = quart) [†]	9.46 × 10 ² cm ³ (0.946 L)
Time	1 min (min = minute)	60 s
	1 h (h = hour)	3600 s
	1 day	86 400 s
Pressure	1 atm (atm = atmosphere)	1.013 25 × 10 ⁵ Pa
	1.000 Torr or 1.000 mmHg	133.3 Pa
	1.000 psi (psi = pounds per square inch)	6.895 kPa
	1 bar	10 ⁵ Pa
Energy	1 cal	4.184 J
	1 eV	1.602 18 × 10 ⁻¹⁹ J; 96.485 kJ·mol ⁻¹
	1 C·V	1 J
	1 kWh (kWh = kilowatt hour)	3.600 × 10 ³ kJ
	1 L·atm	101.325 J
Temperature conversions	(Fahrenheit temperature)/°F = $\frac{9}{5} \times$ (Celsius temperature)/°C + 32	
	(Celsius temperature)/°C = $\frac{5}{9} \times$ {(Fahrenheit temperature)/°F - 32}	
	(Kelvin temperature)/K = (Celsius temperature)/°C + 273.15	

*Entries in boldface type are exact.

[†]The European and Canadian Imperial quart and gallon are 1.201 times as large.

KEY EQUATIONS

1. General

Roots of the equation $ax^2 + bx + c = 0$:

$$x = \frac{-b \pm (b^2 - 4ac)^{1/2}}{2a}$$

Kinetic energy of a particle:

$$E_K = \frac{1}{2}mv^2$$

Gravitational potential energy:

$$E_p = mgh$$

Coulomb potential energy of two charges q_1 and q_2 at a separation r :

$$E_p = q_1q_2/4\pi\epsilon_0r$$

2. Structure and spectroscopy

Relation between the wavelength, λ , and frequency, ν , of electromagnetic radiation:

$$\lambda\nu = c$$

Energy of a photon of electromagnetic radiation of frequency ν :

$$E = h\nu$$

de Broglie equation:

$$\lambda = h/p$$

Heisenberg uncertainty principle:

$$\Delta p\Delta x \geq \frac{1}{2}\hbar$$

Energy of a particle of mass m in a one-dimensional box of length L :

$$E_n = n^2h^2/8mL^2 \quad n = 1, 2, \dots$$

Bohr frequency condition:

$$h\nu = E_{\text{upper}} - E_{\text{lower}}$$

Energy levels of a hydrogenlike atom of atomic number Z :

$$E_n = -Z^2hR/n^2, \quad n = 1, 2, \dots$$

Formal charge

$$FC = V - (L + \frac{1}{2}S)$$

3. Thermodynamics

Ideal gas law:

$$PV = nRT$$

Expansion work against constant external pressure:

$$w = -P_{\text{ex}}\Delta V$$

Work of reversible, isothermal expansion of an ideal gas:

$$w = -nRT \ln(V_{\text{final}}/V_{\text{initial}})$$

First law of thermodynamics:

$$\Delta U = q + w$$

Definition of entropy change:

$$\Delta S = q_{\text{rev}}/T$$

Definition of enthalpy and Gibbs free energy

$$H = U + PV \quad G = H - TS$$

Change in Gibbs free energy at constant temperature:

$$\Delta G = \Delta H - T\Delta S$$

Relation between the constant-pressure and constant-volume molar heat capacities of an ideal gas:

$$C_{P,m} = C_{V,m} + R$$

Standard reaction enthalpy ($X = H$) and Gibbs free energy ($X = G$) from standard enthalpies of formation:

$$\Delta X^\circ = \sum n\Delta X_f^\circ(\text{products}) - \sum n\Delta X_f^\circ(\text{reactants})$$

Standard reaction entropy:

$$\Delta S^\circ = \sum nS_m^\circ(\text{products}) - \sum nS_m^\circ(\text{reactants})$$

Kirchhoff's law:

$$\Delta H_2^\circ = \Delta H_1^\circ + \Delta C_p(T_2 - T_1)$$

Change in entropy when a substance of constant heat capacity, C , is heated from T_1 to T_2 :

$$\Delta S = nR \ln(T_2/T_1)$$

Change in entropy when an ideal gas expands isothermally from V_1 to V_2 :

$$\Delta S = nR \ln(V_2/V_1)$$

Boltzmann's formula for the statistical entropy:

$$S = k \ln W$$

Entropy change of the surroundings for a process in a system with enthalpy change ΔH :

$$\Delta S_{\text{surr}} = -\Delta H/T$$

4. Equilibrium and electrochemistry

Definition of activity:

For an ideal gas: $a_j = P_j/P^\circ$, $P^\circ = 1 \text{ bar}$

For a solute in an ideal solution: $a_j = [j]/c^\circ$, $c^\circ = 1 \text{ mol}\cdot\text{L}^{-1}$

For a pure liquid or solid: $a_j = 1$

Reaction quotient and equilibrium constant:

For the reaction $a A + b B \longrightarrow c C + d D$, $Q = a_C^c a_D^d / a_A^a a_B^b$

For the equilibrium $a A + b B \rightleftharpoons c C + d D$,
 $K = (a_C^c a_D^d / a_A^a a_B^b)_{\text{equilibrium}}$

Variation of Gibbs free energy of reaction with composition:

$$\Delta G_r = \Delta G_r^\circ + RT \ln Q$$

Relation between standard reaction Gibbs free energy and equilibrium constant:

$$\Delta G_r^\circ = -RT \ln K$$

van 't Hoff equation:

$$\ln \frac{K_2}{K_1} = \frac{\Delta H_r^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

Relation between K and K_c :

$$K = (RTc^\circ/P^\circ)^{\Delta n_{\text{gas}}} K_c \quad P^\circ/Rc^\circ = 12.03 \text{ K}$$

Clausius–Clapeyron equation:

$$\ln \frac{P_2}{P_1} = \frac{\Delta H_{\text{vap}}^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

Relation between Gibbs free energy and maximum nonexpansion work:

$$\Delta G = w_{e,\text{max}} \text{ at constant temperature and pressure}$$

Relation between pH and pOH:

$$\text{pH} + \text{pOH} = \text{p}K_w$$

Relation between acidity and basicity constants of a conjugate acid–base pair:

$$\text{p}K_a + \text{p}K_b = \text{p}K_w$$

Henderson–Hasselbalch equation:

$$\text{pH} = \text{p}K_a + \log ([\text{base}]_{\text{initial}} / [\text{acid}]_{\text{initial}})$$

Relation between the Gibbs free energy of reaction and the emf of a cell:

$$\Delta G = -nFE$$

Relation between the equilibrium constant for a cell reaction and the emf of a cell:

$$\ln K = nFE^\circ/RT$$

Nernst equation:

$$E = E^\circ - (RT/nF) \ln Q$$

5. Kinetics

Average reaction rate:

$$\text{Rate of disappearance of R} = -\frac{\Delta[\text{R}]}{\Delta t}$$

$$\text{Rate of formation of P} = \frac{\Delta[\text{P}]}{\Delta t}$$

Unique average rate for $a A + b B \longrightarrow c C + d D$

$$\text{Unique average reaction rate} = -\frac{1}{a} \frac{\Delta[\text{A}]}{\Delta t} = -\frac{1}{b} \frac{\Delta[\text{B}]}{\Delta t} = \frac{1}{c} \frac{\Delta[\text{C}]}{\Delta t} = \frac{1}{d} \frac{\Delta[\text{D}]}{\Delta t}$$

Integrated rate laws:

For Rate of disappearance of $A = k[A]$, $\ln \frac{[A]_t}{[A]_0} = -kt$, $[A]_t = [A]_0 e^{-kt}$

For Rate of disappearance of $A = k[A]^2$,

$$\frac{1}{[A]_t} - \frac{1}{[A]_0} = kt, \quad [A]_t = \frac{[A]_0}{1 + [A]_0 kt}, \quad \frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$$

Half-life of a reactant in a first-order reaction:

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KEY EQUATIONS

1. General

Roots of the equation $ax^2 + bx + c = 0$:

$$x = \frac{-b \pm (b^2 - 4ac)^{1/2}}{2a}$$

Kinetic energy of a particle:

$$E_K = \frac{1}{2}mv^2$$

Gravitational potential energy:

$$E_p = mgh$$

Coulomb potential energy of two charges q_1 and q_2 at a separation r :

$$E_p = q_1q_2/4\pi\epsilon_0r$$

2. Structure and spectroscopy

Relation between the wavelength, λ , and frequency, ν , of electromagnetic radiation:

$$\lambda\nu = c$$

Energy of a photon of electromagnetic radiation of frequency ν :

$$E = h\nu$$

de Broglie equation:

$$\lambda = h/p$$

Heisenberg uncertainty principle:

$$\Delta p\Delta x \geq \frac{1}{2}\hbar$$

Energy of a particle of mass m in a one-dimensional box of length L :

$$E_n = n^2h^2/8mL^2 \quad n = 1, 2, \dots$$

Bohr frequency condition:

$$h\nu = E_{\text{upper}} - E_{\text{lower}}$$

Energy levels of a hydrogenlike atom of atomic number Z :

$$E_n = -Z^2hR/n^2, \quad n = 1, 2, \dots$$

Formal charge

$$FC = V - (L + \frac{1}{2}S)$$

3. Thermodynamics

Ideal gas law:

$$PV = nRT$$

Expansion work against constant external pressure:

$$w = -P_{\text{ex}}\Delta V$$

Work of reversible, isothermal expansion of an ideal gas:

$$w = -nRT \ln(V_{\text{final}}/V_{\text{initial}})$$

First law of thermodynamics:

$$\Delta U = q + w$$

Definition of entropy change:

$$\Delta S = q_{\text{rev}}/T$$

Definition of enthalpy and Gibbs free energy

$$H = U + PV \quad G = H - TS$$

Change in Gibbs free energy at constant temperature:

$$\Delta G = \Delta H - T\Delta S$$

Relation between the constant-pressure and constant-volume molar heat capacities of an ideal gas:

$$C_{p,m} = C_{v,m} + R$$

Standard reaction enthalpy ($X = H$) and Gibbs free energy

($X = G$) from standard enthalpies of formation:

$$\Delta X^\circ = \sum n\Delta X_f^\circ(\text{products}) - \sum n\Delta X_f^\circ(\text{reactants})$$

Standard reaction entropy:

$$\Delta S^\circ = \sum nS_m^\circ(\text{products}) - \sum nS_m^\circ(\text{reactants})$$

Kirchhoff's law:

$$\Delta H_2^\circ = \Delta H_1^\circ + \Delta C_p(T_2 - T_1)$$

Change in entropy when a substance of constant heat capacity, C , is heated from T_1 to T_2 :

$$\Delta S = nR \ln(T_2/T_1)$$

Change in entropy when an ideal gas expands isothermally from V_1 to V_2 :

$$\Delta S = nR \ln(V_2/V_1)$$

Boltzmann's formula for the statistical entropy:

$$S = k \ln W$$

Entropy change of the surroundings for a process in a system with enthalpy change ΔH :

$$\Delta S_{\text{surr}} = -\Delta H/T$$

4. Equilibrium and electrochemistry

Definition of activity:

For an ideal gas: $a_j = P_j/P^\circ$, $P^\circ = 1 \text{ bar}$

For a solute in an ideal solution: $a_j = [j]/c^\circ$, $c^\circ = 1 \text{ mol}\cdot\text{L}^{-1}$

For a pure liquid or solid: $a_j = 1$

Reaction quotient and equilibrium constant:

For the reaction $aA + bB \longrightarrow cC + dD$, $Q = a_C^c a_D^d / a_A^a a_B^b$

For the equilibrium $aA + bB \rightleftharpoons cC + dD$, $K = (a_C^c a_D^d / a_A^a a_B^b)_{\text{equilibrium}}$

Variation of Gibbs free energy of reaction with composition:

$$\Delta G_r = \Delta G_r^\circ + RT \ln Q$$

Relation between standard reaction Gibbs free energy and equilibrium constant:

$$\Delta G_r^\circ = -RT \ln K$$

van 't Hoff equation:

$$\ln \frac{K_2}{K_1} = \frac{\Delta H_r^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

Relation between K and K_c :

$$K = (RTc^\circ/P^\circ)^{\Delta n_{\text{gas}}} K_c \quad P^\circ/Rc^\circ = 12.03 \text{ K}$$

Clausius-Clapeyron equation:

$$\ln \frac{P_2}{P_1} = \frac{\Delta H_{\text{vap}}^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

Relation between Gibbs free energy and maximum nonexpansion work:

$$\Delta G = w_{e,\text{max}} \text{ at constant temperature and pressure}$$

Relation between pH and pOH:

$$\text{pH} + \text{pOH} = \text{p}K_w$$

Relation between acidity and basicity constants of a conjugate acid-base pair:

$$\text{p}K_a + \text{p}K_b = \text{p}K_w$$

Henderson-Hasselbalch equation:

$$\text{pH} = \text{p}K_a + \log \left(\frac{[\text{base}]_{\text{initial}}}{[\text{acid}]_{\text{initial}}} \right)$$

Relation between the Gibbs free energy of reaction and the emf of a cell:

$$\Delta G = -nFE$$

Relation between the equilibrium constant for a cell reaction and the emf of a cell:

$$\ln K = nFE^\circ/RT$$

Nernst equation:

$$E = E^\circ - (RT/nF) \ln Q$$

5. Kinetics

Average reaction rate:

$$\text{Rate of disappearance of R} = -\frac{\Delta[R]}{\Delta t}$$

$$\text{Rate of formation of P} = \frac{\Delta[P]}{\Delta t}$$

Unique average rate for $aA + bB \longrightarrow cC + dD$,

Unique average reaction rate =

$$-\frac{1}{a} \frac{\Delta[A]}{\Delta t} = -\frac{1}{b} \frac{\Delta[B]}{\Delta t} = \frac{1}{c} \frac{\Delta[C]}{\Delta t} = \frac{1}{d} \frac{\Delta[D]}{\Delta t}$$

Integrated rate laws:

For Rate of disappearance of $A = k[A]$, $\ln \frac{[A]_t}{[A]_0} = -kt$, $[A]_t = [A]_0 e^{-kt}$

For Rate of disappearance of $A = k[A]^2$,

$$\frac{1}{[A]_t} - \frac{1}{[A]_0} = kt, \quad [A]_t = \frac{[A]_0}{1 + [A]_0 kt}, \quad \frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$$

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THE ELEMENTS

Element	Symbol	Atomic number	Molar mass* (g·mol ⁻¹)	Element	Symbol	Atomic number	Molar mass* (g·mol ⁻¹)
Actinium	Ac	89	(227)	Mendelevium	Md	101	(258)
Aluminum	Al	13	26.98	Mercury	Hg	80	200.59
Americium	Am	95	(243)	Molybdenum	Mo	42	95.94
Antimony	Sb	51	121.76	Neodymium	Nd	60	144.24
Argon	Ar	18	39.95	Neon	Ne	10	20.18
Arsenic	As	33	74.92	Neptunium	Np	93	(237)
Astatine	At	85	(210)	Nickel	Ni	28	58.69
Barium	Ba	56	137.33	Niobium	Nb	41	92.91
Berkelium	Bk	97	(247)	Nitrogen	N	7	14.01
Beryllium	Be	4	9.01	Nobelium	No	102	(259)
Bismuth	Bi	83	208.98	Osmium	Os	76	190.23
Bohrium	Bh	107	(264)	Oxygen	O	8	16.00
Boron	B	5	10.81	Palladium	Pd	46	106.42
Bromine	Br	35	79.90	Phosphorus	P	15	30.97
Cadmium	Cd	48	112.41	Platinum	Pt	78	195.08
Calcium	Ca	20	40.08	Plutonium	Pu	94	(244)
Californium	Cf	98	(251)	Polonium	Po	84	(209)
Carbon	C	6	12.01	Potassium	K	19	39.10
Cerium	Ce	58	140.12	Praseodymium	Pr	59	140.91
Cesium	Cs	55	132.91	Promethium	Pm	61	(145)
Chlorine	Cl	17	35.45	Protactinium	Pa	91	231.04
Chromium	Cr	24	52.00	Radium	Ra	88	(226)
Cobalt	Co	27	58.93	Radon	Rn	86	(222)
Copper	Cu	29	63.55	Rhenium	Re	75	186.21
Curium	Cm	96	(247)	Rhodium	Rh	45	102.90
Darmstadtium	Ds	110	—	Roentgenium	Rg	111	—
Dubnium	Db	105	(262)	Rubidium	Rb	37	85.47
Dysprosium	Dy	66	162.50	Ruthenium	Ru	44	101.07
Einsteinium	Es	99	(252)	Rutherfordium	Rf	104	(261)
Erbium	Er	68	167.26	Samarium	Sm	62	150.36
Europium	Eu	63	151.96	Scandium	Sc	21	44.96
Fermium	Fm	100	(257)	Seaborgium	Sg	106	(266)
Fluorine	F	9	19.00	Selenium	Se	34	78.96
Francium	Fr	87	(223)	Silicon	Si	14	28.09
Gadolinium	Gd	64	157.25	Silver	Ag	47	107.87
Gallium	Ga	31	69.72	Sodium	Na	11	22.99
Germanium	Ge	32	72.64	Strontium	Sr	38	87.62
Gold	Au	79	196.97	Sulfur	S	16	32.06
Hafnium	Hf	72	178.49	Tantalum	Ta	73	180.95
Hassium	Hs	108	(277)	Technetium	Tc	43	(98)
Helium	He	2	4.00	Tellurium	Te	52	127.60
Holmium	Ho	67	164.93	Terbium	Tb	65	158.93
Hydrogen	H	1	1.0079	Thallium	Tl	81	204.38
Indium	In	49	114.82	Thorium	Th	90	232.04
Iodine	I	53	126.90	Thulium	Tm	69	168.93
Iridium	Ir	77	192.22	Tin	Sn	50	118.71
Iron	Fe	26	55.84	Titanium	Ti	22	47.87
Krypton	Kr	36	83.80	Tungsten	W	74	183.84
Lanthanum	La	57	138.91	Uranium	U	92	238.03
Lawrencium	Lr	103	(262)	Vanadium	V	23	50.94
Lead	Pb	82	207.2	Xenon	Xe	54	131.29
Lithium	Li	3	6.94	Ytterbium	Yb	70	173.04
Lutetium	Lu	71	174.97	Yttrium	Y	39	88.91
Magnesium	Mg	12	24.31	Zinc	Zn	30	65.41
Manganese	Mn	25	54.94	Zirconium	Zr	40	91.22
Meitnerium	Mt	109	(268)				

*Parentheses around molar mass indicate the most stable isotope of a radioactive element.

SI PREFIXES

FUNDAMENTAL CONSTANTS

	Name	Symbol	Value
z	Atomic mass constant	m_u	$1.660\ 54 \times 10^{-27}$ kg
zepto- 10^{-21}	Avogadro's constant	N_A	$6.022\ 14 \times 10^{23}$ mol ⁻¹
a	Boltzmann's constant	k	$1.380\ 66 \times 10^{-23}$ J·K ⁻¹
atto- 10^{-18}	Fundamental charge	e	$1.602\ 18 \times 10^{-19}$ C
f	Faraday's constant	$F = N_A e$	$9.648\ 53 \times 10^4$ C·mol ⁻¹
femto 10^{-15}	Gas constant	$R = N_A k$	$8.314\ 47$ J·K ⁻¹ ·mol ⁻¹ $8.314\ 47$ L·kPa·K ⁻¹ ·mol ⁻¹ $8.205\ 74 \times 10^{-2}$ L·atm·K ⁻¹ ·mol ⁻¹ $62.36\ 37$ L·Torr·K ⁻¹ ·mol ⁻¹ $8.314\ 47 \times 10^{-2}$ L·bar·K ⁻¹ ·mol ⁻¹
p	Mass of electron	m_e	$9.109\ 38 \times 10^{-31}$ kg
pico- 10^{-12}	Mass of neutron	m_n	$1.674\ 93 \times 10^{-27}$ kg
n	Mass of proton	m_p	$1.672\ 62 \times 10^{-27}$ kg
nano- 10^{-9}	Planck's constant	h	$6.626\ 08 \times 10^{-34}$ J·s
μ	Rydberg constant	$\hbar = h/2\pi$	$1.054\ 57 \times 10^{-34}$ J·s
micro- 10^{-6}	Speed of light	c	$3.289\ 84 \times 10^{15}$ Hz
m	Standard acceleration of free fall	g	$2.997\ 92 \times 10^8$ m·s ⁻¹
milli- 10^{-3}	Vacuum permittivity	ϵ_0	$9.806\ 65$ m·s ⁻² $8.854\ 19 \times 10^{-12}$ J ⁻¹ ·C ² ·m ⁻¹

RELATIONS BETWEEN UNITS*

	Property	Common unit	SI unit
c	Mass	2.205 lb (lb = pound)	1.000 kg
centi- 10^{-2}		1.000 lb	453.6 g
d		1.000 oz (oz = ounce)	28.35 g
deci- 10^{-1}		1.000 ton (= 2000 lb)	907.2 kg
deka- 10		1 t (t = tonne, metric ton)	10 ³ kg
h	Length	1.094 yd (yd = yard)	1.000 m
hecto- 10^2		0.3937 in. (in. = inch)	1.000 cm
k		0.6214 mi (mi = mile)	1.000 km
kilo- 10^3		1 in.	2.54 cm
M		1 ft (ft = foot)	30.48 cm
mega- 10^6	Volume	1.000 yd	0.9144 m
G		1 Å (Å = ångström)	10 ⁻¹⁰ m
giga- 10^9		1 L (L = liter)	10 ³ cm ³ , 1 dm ³
T		1.000 gal (gal = gallon) [†]	3.785 dm ³ (3.785 L)
tera- 10^{12}		1.00 ft ³ (ft ³ = cubic foot)	2.83 × 10 ⁻² m ³ (28.3 L)
		1.00 qt (qt = quart) [†]	9.46 × 10 ² cm ³ (0.946 L)
	Time	1 min (min = minute)	60 s
		1 h (h = hour)	3600 s
		1 day	86 400 s
	Pressure	1 atm (atm = atmosphere)	1.013 25 × 10 ⁵ Pa
		1.000 Torr or 1.000 mmHg	133.3 Pa
		1.000 psi (psi = pounds per square inch)	6.895 kPa
		1 bar	10 ⁵ Pa
	Energy	1 cal	4.184 J
		1 eV	1.602 18 × 10 ⁻¹⁹ J; 96.485 kJ·mol ⁻¹
		1 C·V	1 J
		1 kWh (kWh = kilowatt hour)	3.600 × 10 ³ kJ
		1 L·atm	101.325 J
	Temperature conversions	(Fahrenheit temperature)/°F = $\frac{9}{5} \times$ (Celsius temperature)/°C + 32 (Celsius temperature)/°C = $\frac{5}{9} \times$ {(Fahrenheit temperature)/°F - 32} (Kelvin temperature)/K = (Celsius temperature)/°C + 273.15	

*Entries in boldface type are exact.

[†]The European and Canadian Imperial quart and gallon are 1.201 times as large.

LETTER FROM THE AUTHORS

Dear Colleagues,

We are pleased to present this new edition of our textbook, *Chemical Principles: The Quest for Insight*. It is designed for a rigorous course in introductory chemistry and to appeal to those of your students who will focus on engineering, the life sciences and medicine, or environmental sciences, as well as to chemistry majors.

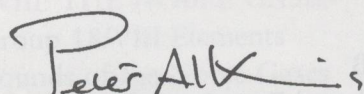
Chemical Principles encourages students to question and to develop insight by emphasizing the nature of chemistry and how chemical knowledge is obtained and developed. We have retained the overall structure of the text, which has been so well received. It begins with a review of the basics in the Fundamentals sections, which instructors have used in a variety of ways. In the main body of the book an “atoms-first” organization introduces students to the most basic structure of matter before building on this knowledge to develop more complex properties and interactions.

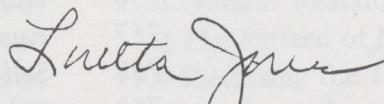
With this new edition, we have paid particular attention to three areas: problem solving, the interpretation of mathematical expressions, and encouraging good practice. The most prominent new feature is “Picture the process,” the thumbnail illustrations that accompany the steps in most worked Examples and some derivations. These little illustrations serve several purposes. On one hand they will make the text more accessible to a wider range of students; on the other hand, they will encourage students taking higher-level courses to stop and think about what they are doing. They will also help all students make connections between the various representations of chemistry, such as graphs, equations, and molecular structures. In the new “What does this equation mean” feature we walk the reader through the symbols in a mathematical expression, encouraging them to listen to what it is saying. In the new “Notes on good practice” feature we explain common pitfalls and encourage students to express themselves precisely. We have acknowledged—with enthusiasm—the rising interest in nanotechnology and green chemistry and have responded to the request for a wider range of higher-level exercises.

We have paid particular attention to maintaining the length of the text: what growth there has been is due entirely to the additional pedagogical features, such as “Picture the process,” that we have introduced to reduce the cognitive load of the material for the reader. A few of the less central topics and some with burdensome mathematics have been moved to the book’s Web site.

We are gratified by the response to the first three editions of this book. Our thanks go to all who have provided feedback: we listened carefully to your comments as we prepared this new edition. We hope that you find it an interesting, dynamic, and interactive textbook for the modern student and instructor, with innovative pedagogical features. We look forward very much to hearing from you about it.

Yours sincerely,


Peter Atkins


Loretta Jones