Chemistry Data Book

Second Edition in SI

Compiled by

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Foreword by

M. L. McGlashan Ph.D., D.Sc., C.Chem., F.R.S.C.

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Preface

Since the SI edition of this book was published in 1970, the chemical nomenclature (particularly for organic compounds) has been extensively revised, minor changes have been made to the data in various tables and an index has been added. In this new edition the opportunity has been taken to correct some remaining errors, update the data and delete a number of tables which are no longer relevant to the majority of A-level syllabuses.

The following tables have been added for this edition:

Equilibrium constants for gaseous reactions at various temperatures
Electrolytic conductivity of water at various temperatures
Infrared data.

In addition Gibbs free energies of formation of aqueous ions have been included in Table 32 and the table of lattice enthalpies has been extended to include theoretical values.

The use of data in the teaching of chemistry has become increasingly important in recent years and the authors' intention remains to provide a book which will be used as a comprehensive source of the chemical data which are likely to be needed by sixth-form and technical college students and first-year university students. It is hoped that the book will be used not only for reference, but also in the discussion of problems and ideas arising from practical work. The general layout of the tables is as follows:

physical constants and fundamental particles
the elements
basic atomic and molecular properties
thermodynamic properties
kinetic data
organic data
analytical data
miscellaneous data.

The detailed list of contents should enable the reader to find the data he or she needs quite easily. There is also an index at the end of the book. Many of the tables are preceded by a brief explanation of the data contained in them.

The compilers would welcome any constructive criticisms and suggestions from readers which will increase the usefulness of the book.

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J. G. Stark
H. G. Wallace

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The authors wish to acknowledge the many sources used in the compilation of this data book and particularly the following:

F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry* (Interscience, New York, 2nd edn., 1966).

Chemical Bond Approach Committee, *Chemical Systems* (McGraw-Hill, New York, 1964).

K. B. Harvey and G. B. Porter, *Physical Inorganic Chemistry* (Addison-Wesley, Reading, Mass., 1963).

W. M. Latimer, *Oxidation Potentials* (Prentice-Hall, Englewood Cliffs, New Jersey, 2nd edn., 1952).

T. Moeller, *Inorganic Chemistry* (Wiley, New York, 1952).

Periodic Table of the Elements and *Table of Periodic Properties of the Elements* (E. H. Sargent and Co.).

R. C. Weast (ed.), *Handbook of Chemistry and Physics* (Chemical Rubber Co., 47th edn., 1966).

They are also grateful to Professor M. L. McGlashan for his advice and criticism and for writing a foreword to the book and to Dr A. D. Pethybridge, of the University of Reading, for his helpful suggestions in relation to Table 1.

Foreword

The metric system of units had 'just grown', since the Metre Convention of 1875, until it contained many redundant units. For example the joule, the erg, the kilogram-force metre, the kilowatt hour, the electronvolt, at least three calories differing from one another by as much as one part in a thousand, the thermie, and the litre atmosphere, were all used as units of energy in 'metric' countries and by scientists everywhere. To these, Anglo-Saxon technologists added the poundal, the foot pound-force, the British thermal unit, and the horsepower hour.

In 1960 a small but sufficient set of metric units was carefully chosen by the General Conference on Weights and Measures and given the name *SI Units*, and these together with their decimal multiples and sub-multiples formed by use of the *SI Prefixes,* became the *International System of Units (SI)*. The adoption of the SI has been strongly urged on the scientific and technological world by the International Organization for Standardization and by the International Scientific Unions including that of Pure and Applied Chemistry, and it is in fact rapidly being adopted throughout the scientific literature. It has already been adopted in several major countries as the only legal system of weights and measures for purposes of trade, and is about to be adopted in many more.

If the United Kingdom were already 'metric' (as we so nearly were in 1871 when a Bill for the compulsory adoption of the metric system was defeated by only five votes on its Second Reading in the House of Commons) then we should no doubt now be in the process of 'going SI'. By luck the SI was ready for us when in 1965 we were at last ready to take the decision to 'go metric'. According to the Government's Metrication programme 1975 was the deadline by which the SI should have been adopted throughout the Nation's industry, commerce, and daily life. That target was not reached but nevertheless steady progress is being made.

Students of chemistry must learn to use the SI and, more importantly, to 'think SI', whatever their future careers may be.

Mr Stark and Mr Wallace have served chemists and chemistry well by producing their book, which contains a most useful collection of the results of physicochemically important measurements expressed as the numbers which are equal to the ratios of a physical quantity and an appropriate SI unit.

M. L. McGlashan

Thermodynamic Sign Convention

All thermodynamic data in this book refer to the standard temperature of 298 K. The sign convention used is that ΔH denotes the difference between the final and the initial enthalpy, i.e. $\Delta H = H_f - H_i$.

SI Units

There are seven *basic SI units* as shown in Table I.

Table I **Basic SI Units**

Physical quantity	*Name of unit*	*Symbol*
Length	metre	m
Mass	kilogram	kg
Time	second	s
Electric current	ampere	A
Thermodynamic temperature	kelvin (*not* degree Kelvin)	K (*not* °K)
Luminous intensity	candela	cd
Amount of substance	mole	mol

In addition, there are *derived units* which are defined in terms of the basic units or other derived units. Some of those most likely to be met by the user of this book are shown in Table II.

Table II **Derived Units**

Physical quantity	*Name of unit*	*Symbol and definition*
Force	newton	N ($kg\ m\ s^{-2} = J\ m^{-1}$)
Energy, heat	joule	J ($kg\ m^2\ s^{-2}$)
Power	watt	W ($kg\ m^2\ s^{-3} = J\ s^{-1}$)
Electric charge	coulomb	C (A s)
Electric potential difference	volt	V ($kg\ m^2\ s^{-3}\ A^{-1} = J\ A^{-1}\ s^{-1}$)
Electric resistance	ohm	Ω ($kg\ m^2\ s^{-3}\ A^{-2} = V\ A^{-1}$)
Electric capacitance	farad	F ($A^2\ s^4\ kg^{-1}\ m^{-2} = A\ s\ V^{-1}$)
Magnetic flux	weber	Wb ($kg\ m^2\ s^{-2}\ A^{-1} = V\ s$)
Magnetic flux density	tesla	T ($kg\ s^{-2}\ A^{-1} = V\ s\ m^{-2}$)
Inductance	henry	H ($kg\ m^2\ s^{-2}\ A^{-2} = V\ s\ A^{-1}$)
Frequency	hertz	Hz (s^{-1})

There are also derived units, such as those of volume, density, pressure and specific heat capacity, which are based on SI units. The names and symbols of these units are derived from those in Tables I and II as shown in Table III.

Table III **Other Derived Units Based on SI**

Physical quantity	*Name of unit*	*Symbol*	
Area	square metre	m^2	
Volume	cubic metre	m^3	
Velocity	metre per second	$m\ s^{-1}$	
Acceleration	metre per second squared	$m\ s^{-2}$	
Density	kilogram per cubic metre	$kg\ m^{-3}$	
Pressure	newton per square metre (pascal)	$N\ m^{-2}$ (Pa)	$kg\ m^{-1}\ s^{-2}$
Surface tension	newton per metre	$N\ m^{-1}$	$kg\ s^{-2}$
Electric field strength	volt per metre	$V\ m^{-1}$	$kg\ m\ s^{-3}\ A^{-1}$
Magnetic field strength	ampere per metre	$A\ m^{-1}$	
Dipole moment	coulomb metre	C m	A s m
Magnetic moment	ampere square metre	$A\ m^2$	
Heat capacity, Entropy	joule per kelvin	$J\ K^{-1}$	$kg\ m^2\ s^{-2}\ K^{-1}$
Specific heat capacity	joule per kilogram kelvin	$J\ kg^{-1}\ K^{-1}$	$m^2\ s^{-2}\ K^{-1}$
Concentration	mole per cubic metre	$mol\ m^{-3}$	

Multiples of units in powers of ten are indicated by means of agreed prefixes and symbols as shown in Table IV.

Table IV **Multiples of Units**

Multiple	*Prefix*	*Symbol*	*Multiple*	*Prefix*	*Symbol*
10^{12}	tera	T	10^{-1}	deci	d
10^{9}	giga	G	10^{-2}	centi	c
10^{6}	mega	M	10^{-3}	milli	m
10^{3}	kilo	k	10^{-6}	micro	μ
10^{2}	hecto	h	10^{-9}	nano	n
10	deca	da	10^{-12}	pico	p

Details of SI units can be found in the following publications:

The International System (SI) Units (B.S. 3763), British Standards Institution, 1970.

M. L. McGlashan, *Physico-Chemical Quantities and Units*, 2nd edn, Royal Institute of Chemistry, 1971.

Quantities, Units, and Symbols, The Royal Society, 1971.

Contents

1 Physical Constants and Conversion Factors

Speed of light in a vacuum (c) = $2{\cdot}997\,925 \times 10^{8}$ m s^{-1}
Boltzmann constant (k) = $1{\cdot}380\,662 \times 10^{-23}$ J K^{-1}
Planck constant (h) = $6{\cdot}626\,176 \times 10^{-34}$ J s
Rydberg constant (R_H) = $1{\cdot}097\,373 \times 10^{7}$ m^{-1}
Avogadro constant (L) = $6{\cdot}022\,045 \times 10^{23}$ mol^{-1}
Gas constant (R) = $8{\cdot}314\,41$ J K^{-1} mol^{-1}
= $1{\cdot}987\,1$ cal K^{-1} mol^{-1}
= $82{\cdot}053$ cm^{3} atm K^{-1} mol^{-1}
'Ice-point' temperature (T_{ice}) = $273{\cdot}150\,0$ K
Faraday constant (F) = $9{\cdot}648\,456 \times 10^{4}$ C mol^{-1}

Molar volume of an ideal gas at s.t.p.[a] ($V_m^{\ominus}$) = $2{\cdot}241\,383 \times 10^{-2}$ m^{3} mol^{-1}
Triple point temperature of water = $273{\cdot}16$ K
Potential of a standard Weston cell (saturated) at θ_C
= $[1{\cdot}018\,3 - 4 \times 10^{-5}(\theta_C/^{\circ}C - 20)]$V

Nernst factor $\left(\dfrac{RT\ln 10}{F}\right)$ at 25 °C = $0{\cdot}059\,159$ V

1 calorie (cal) = $4{\cdot}184$ J
1 electrostatic unit of charge $\hat{=}$ $3{\cdot}335\,640 \times 10^{-10}$ C
L eV[b] $\hat{=}$ $96{\cdot}484$ kJ mol^{-1}
1 atmosphere (atm) = 760 torr ($\approx$ 760 mmHg) = 101 325 N m^{-2} (Pa)
1 ångström (Å) = 10^{-10} m = 10^{-8} cm = 10^{-4} µm
= 10^{-1} nm = 10^{2} pm
1 litre (l) = 10^{-3} m^{3} = 1 dm^{3} = 10^{3} cm^{3}
1 curie (Ci) = $3{\cdot}7 \times 10^{10}$ s^{-1}
Conversion of Celsius temperature to thermodynamic temperature:
$\theta_C/^{\circ}C = T/K - 273{\cdot}150$
$\ln x = 2{\cdot}303 \log_{10} x$

2 Fundamental Particles

	Proton	*Neutron*	*Electron*
Symbol	p	n	e
Mass	$1{\cdot}672\,648 \times 10^{-27}$ kg	$1{\cdot}674\,954 \times 10^{-27}$ kg	$9{\cdot}109\,534 \times 10^{-31}$ kg
Charge	$1{\cdot}602\,189 \times 10^{-19}$ C	0	$1{\cdot}602\,189 \times 10^{-19}$ C
Mass relative to electron	1836	1839	1
Charge relative to proton	+1	0	−1

[a] That is 273·15 K and 101 325 N m^{-2} pressure.
[b] The quantity L eV is commonly, but incorrectly, known as an 'electronvolt'.

3 The Electromagnetic Spectrum

	Wavelength		*Wave number*	*Frequency*	*Energy quantum*	
	λ/m	λ	σ/m^{-1}	ν/MHz	$Lh\nu/\mathrm{kJ\ mol}^{-1}$	$Lh\nu/\mathrm{eV\ mol}^{-1}$
Gamma rays	10^{-12}	10^{-2} Å	10^{12}	$3{\cdot}00 \times 10^{14}$	$1{\cdot}20 \times 10^{8}$	$1{\cdot}24 \times 10^{6}$
X-rays	10^{-10}	1 Å	10^{10}	$3{\cdot}00 \times 10^{12}$	$1{\cdot}20 \times 10^{6}$	$1{\cdot}24 \times 10^{4}$
Ultra-violet	10^{-8}	10^{2} Å	10^{8}	$3{\cdot}00 \times 10^{10}$	$1{\cdot}20 \times 10^{4}$	$1{\cdot}24 \times 10^{2}$
Visible	10^{-6}	1 μm	10^{6}	$3{\cdot}00 \times 10^{8}$	$1{\cdot}20 \times 10^{2}$	1·24
Infra-red	10^{-4}	10^{2} μm	10^{4}	$3{\cdot}00 \times 10^{6}$	1·20	$1{\cdot}24 \times 10^{-2}$
Micro-waves	10^{-2}	10^{4} μm	10^{2}	$3{\cdot}00 \times 10^{4}$	$1{\cdot}20 \times 10^{-2}$	$1{\cdot}24 \times 10^{-4}$
Television waves	1	10^{6} μm	1	$3{\cdot}00 \times 10^{2}$	$1{\cdot}20 \times 10^{-4}$	$1{\cdot}24 \times 10^{-6}$
Radio waves	10^{2}	10^{8} μm	10^{-2}	3·00	$1{\cdot}20 \times 10^{-6}$	$1{\cdot}24 \times 10^{-8}$

The Visible Spectrum

	Wavelength	*Wave number*	*Energy quantum*	
	λ/m	σ/m^{-1}	$Lh\nu/\mathrm{kJ\ mol}^{-1}$	$Lh\nu/\mathrm{eV\ mol}^{-1}$
Violet	$4{\cdot}00 \times 10^{-7}$	$2{\cdot}50 \times 10^{6}$	299	3·10
Blue				
Green	$5{\cdot}00 \times 10^{-7}$	$2{\cdot}00 \times 10^{6}$	239	2·48
Yellow	$5{\cdot}89 \times 10^{-7}$ (sodium D line)			
Orange	$6{\cdot}00 \times 10^{-7}$	$1{\cdot}67 \times 10^{6}$	199	2·06
Red	$7{\cdot}00 \times 10^{-7}$	$1{\cdot}43 \times 10^{6}$	171	1·77

4 The Periodic Classification (with atomic numbers)

Group	I	II																									III	IV	V	VI	VII	VIII
Period																																
1	s-block												1 H	2 He																		
																											p-block					
2	3 Li	4 Be																									5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg																									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
			d-block																			d-block										
4	19 K	20 Ca	21 Sc															22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y															40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
									f-block																							
6	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 –														

5 Electronic Configurations of the Elements (ground states)

Shell		*K*	*L*		*M*			*N*			
	n	*1*	*2*		*3*			*4*			
Atomic number	*Element*	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
1	Hydrogen	1									
2	Helium	2									
3	Lithium	2	1								
4	Beryllium	2	2								
5	Boron	2	2	1							
6	Carbon	2	2	2							
7	Nitrogen	2	2	3							
8	Oxygen	2	2	4							
9	Fluorine	2	2	5							
10	Neon	2	2	6							
11	Sodium	2	2	6	1						
12	Magnesium	2	2	6	2						
13	Aluminium	2	2	6	2	1					
14	Silicon	2	2	6	2	2					
15	Phosphorus	2	2	6	2	3					
16	Sulphur	2	2	6	2	4					
17	Chlorine	2	2	6	2	5					
18	Argon	2	2	6	2	6					
19	Potassium	2	2	6	2	6		1			
20	Calcium	2	2	6	2	6		2			
21	Scandium	2	2	6	2	6	1	2			
22	Titanium	2	2	6	2	6	2	2			
23	Vanadium	2	2	6	2	6	3	2			
24	Chromium	2	2	6	2	6	5	1			
25	Manganese	2	2	6	2	6	5	2			
26	Iron	2	2	6	2	6	6	2			
27	Cobalt	2	2	6	2	6	7	2			
28	Nickel	2	2	6	2	6	8	2			
29	Copper	2	2	6	2	6	10	1			
30	Zinc	2	2	6	2	6	10	2			
31	Gallium	2	2	6	2	6	10	2	1		
32	Germanium	2	2	6	2	6	10	2	2		
33	Arsenic	2	2	6	2	6	10	2	3		
34	Selenium	2	2	6	2	6	10	2	4		
35	Bromine	2	2	6	2	6	10	2	5		
36	Krypton	2	2	6	2	6	10	2	6		

Shell		K	L	M	N				O				P		
		n = 1	2	3	4				5				6		
Atomic number	Element				4s	4p	4d	4f	5s	5p	5d	5f	6s	6p	6d
37	Rubidium	2	8	18	2	6			1						
38	Strontium	2	8	18	2	6			2						
39	Yttrium	2	8	18	2	6	1		2						
40	Zirconium	2	8	18	2	6	2		2						
41	Niobium	2	8	18	2	6	4		1						
42	Molybdenum	2	8	18	2	6	5		1						
43	Technetium	2	8	18	2	6	6		1						
44	Ruthenium	2	8	18	2	6	7		1						
45	Rhodium	2	8	18	2	6	8		1						
46	Palladium	2	8	18	2	6	10								
47	Silver	2	8	18	2	6	10		1						
48	Cadmium	2	8	18	2	6	10		2						
49	Indium	2	8	18	2	6	10		2	1					
50	Tin	2	8	18	2	6	10		2	2					
51	Antimony	2	8	18	2	6	10		2	3					
52	Tellurium	2	8	18	2	6	10		2	4					
53	Iodine	2	8	18	2	6	10		2	5					
54	Xenon	2	8	18	2	6	10		2	6					
55	Caesium	2	8	18	2	6	10		2	6			1		
56	Barium	2	8	18	2	6	10		2	6			2		
57	Lanthanum	2	8	18	2	6	10		2	6	1		2		
58	Cerium	2	8	18	2	6	10	2	2	6			2		
59	Praseodymium	2	8	18	2	6	10	3	2	6			2		
60	Neodymium	2	8	18	2	6	10	4	2	6			2		
61	Promethium	2	8	18	2	6	10	5	2	6			2		
62	Samarium	2	8	18	2	6	10	6	2	6			2		
63	Europium	2	8	18	2	6	10	7	2	6			2		
64	Gadolinium	2	8	18	2	6	10	7	2	6	1		2		
65	Terbium	2	8	18	2	6	10	9	2	6			2		
66	Dysprosium	2	8	18	2	6	10	10	2	6			2		
67	Holmium	2	8	18	2	6	10	11	2	6			2		
68	Erbium	2	8	18	2	6	10	12	2	6			2		
69	Thulium	2	8	18	2	6	10	13	2	6			2		
70	Ytterbium	2	8	18	2	6	10	14	2	6			2		
71	Lutetium	2	8	18	2	6	10	14	2	6	1		2		
72	Hafnium	2	8	18	2	6	10	14	2	6	2		2		
73	Tantalum	2	8	18	2	6	10	14	2	6	3		2		
74	Tungsten	2	8	18	2	6	10	14	2	6	4		2		
75	Rhenium	2	8	18	2	6	10	14	2	6	5		2		
76	Osmium	2	8	18	2	6	10	14	2	6	6		2		
77	Iridium	2	8	18	2	6	10	14	2	6	9				
78	Platinum	2	8	18	2	6	10	14	2	6	9		1		
79	Gold	2	8	18	2	6	10	14	2	6	10		1		
80	Mercury	2	8	18	2	6	10	14	2	6	10		2		
81	Thallium	2	8	18	2	6	10	14	2	6	10		2	1	
82	Lead	2	8	18	2	6	10	14	2	6	10		2	2	
83	Bismuth	2	8	18	2	6	10	14	2	6	10		2	3	
84	Polonium	2	8	18	2	6	10	14	2	6	10		2	4	
85	Astatine	2	8	18	2	6	10	14	2	6	10		2	5	
86	Radon	2	8	18	2	6	10	14	2	6	10		2	6	