

Chemistry data booklet

For use during the course and in the examinations
First assessment 2025

Version 1.1



International Baccalaureate®
Baccalauréat International
Bachillerato Internacional

**Diploma Programme
Chemistry data booklet**

Published February 2023
Updated February 2024

Published by the International Baccalaureate Organization, a not-for-profit educational

foundation of Rue du Pré-de-la-Bichette 1, 1202 Genève, Switzerland.

Website: ibo.org

© International Baccalaureate Organization 2023

The International Baccalaureate Organization (known as the IB) offers four high-quality and challenging educational programmes for a worldwide community of schools, aiming to create a better, more peaceful world. This publication is one of a range of materials produced to support these programmes.

The IB may use a variety of sources in its work and check information to verify accuracy and authenticity, particularly when using community-based knowledge sources such as Wikipedia. The IB respects the principles of intellectual property and makes strenuous efforts to identify and obtain permission before publication from rights holders of all copyright material used. The IB is grateful for permissions received for material used in this publication and will be pleased to correct any errors or omissions at the earliest opportunity.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, without the IB's prior written permission, or as expressly permitted by the [Rules for use of IB Intellectual Property](#).

IB merchandise and publications can be purchased through the [IB Store](#) (email: sales@ibo.org). Any commercial use of IB publications (whether fee-covered or commercial) by third parties acting in the IB's ecosystem without a formal relationship with the IB (including but not limited to tutoring organizations, professional development providers, educational publishers and operators of curriculum mapping or teacher resource digital platforms, etc.) is prohibited and requires a subsequent written licence from the IB. Licence requests should be sent to copyright@ibo.org. More information can be obtained on the [IB public website](#).

Contents

Introduction.....	1
1. Some relevant equations	2
2. Physical constants	3
3. Metric (SI) multipliers	4
4. Unit conversions and standard conditions	5
5. The electromagnetic spectrum	5
6. Names of the elements.....	6
7. The periodic table.....	8
8. Melting points and boiling points of the elements at 101.325 kPa	9
9. First ionization energy, electron affinity and electronegativity of the elements.....	10
10. Atomic and ionic radii of the elements	11
11. Covalent or average covalent bond lengths.....	12
12. Bond enthalpies or average bond enthalpies at 298.15 K	13
13. Thermodynamic data (selected compounds).....	14
14. Enthalpies of combustion	15
15. Colour wheel with wavelengths of the visible spectrum	16
16. Lattice enthalpies at 298.15 K (experimental values)	17
17. Triangular bonding diagram (van Arkel–Ketelaar triangle)	18
18. Acid–base indicators.....	19
19. Standard reduction potentials at 298.15 K	20
20. Infrared data	21
21. ^1H NMR data.....	22
22. Mass spectral fragments lost	23
23. Uncertainties.....	23
24. References	24
Updates to the publication	25

This page is intentionally blank.

Introduction

This Diploma Programme (DP) *Chemistry data booklet* accompanies the DP *Chemistry guide* and DP *Chemistry teacher support material*. It contains chemical and physical equations and constants, chemical symbols, the periodic table, and other chemical data relevant to the course.

Students must have access to a copy of this booklet for the duration of the course, so that they can become familiar with its contents. Direct reference is made to relevant equations in the “Understandings” sections of the guide. This helps to maintain the emphasis on interpretation and application rather than memorization of symbols, constants and equations.

Each student must have access to a clean copy of the *Chemistry data booklet* during examinations. It is the responsibility of the school to download a copy of this booklet from IBIS or the Programme Resource Centre and to ensure that there are sufficient copies available for all students.

1. Some relevant equations

Equation
$c = f\lambda$
$E = hf$
$n = \frac{m}{M}$
$n = CV$
$PV = nRT$
$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$
$Q = mc\Delta T$
% atom economy = $\frac{\text{molar mass of desired product}}{\text{molar mass of all reactants}} \times 100$
$\Delta H^\ominus = \sum(\Delta H_f^\ominus_{\text{products}}) - \sum(\Delta H_f^\ominus_{\text{reactants}})$
$\Delta H^\ominus = \sum(\Delta H_c^\ominus_{\text{reactants}}) - \sum(\Delta H_c^\ominus_{\text{products}})$
$\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$
$\Delta G = \Delta G^\ominus + RT \ln Q$
$\Delta G^\ominus = -RT \ln K$
$\Delta G^\ominus = -nFE^\ominus$
$k = A e^{\frac{-E_a}{RT}}$
$\ln k = \frac{-E_a}{RT} + \ln A$
$\text{pH} = -\log_{10} [\text{H}_3\text{O}^+]$
or
$\text{pH} = -\log_{10} [\text{H}^+]$
$K_w = [\text{H}^+] [\text{OH}^-]$
$\text{pOH} = -\log_{10} [\text{OH}^-]$

2. Physical constants

Quantity	Symbol	Approximate value
Elementary charge	e	1.602177×10^{-19} C
Electron rest mass	m_e	9.109384×10^{-31} kg
Proton rest mass	m_p	1.672622×10^{-27} kg
Neutron rest mass	m_n	1.674927×10^{-27} kg
Speed of light in vacuum	c	3.00×10^8 m s ⁻¹
Planck constant	h	6.63×10^{-34} J s
Avogadro constant	N_A	6.02×10^{23} mol ⁻¹
Gas constant	R	8.31 J K ⁻¹ mol ⁻¹
Molar volume of an ideal gas at STP	V_m	2.27×10^{-2} m ³ mol ⁻¹ = 22.7 dm ³ mol ⁻¹
Specific heat capacity of water	c_w	4.18 kJ kg ⁻¹ K ⁻¹ = 4.18 J g ⁻¹ K ⁻¹
Ionic product constant for water at 298.15 K	K_w	1.00×10^{-14} mol ² dm ⁻⁶
Faraday constant	F	9.65×10^4 C mol ⁻¹

3. Metric (SI) multipliers

Prefix	Abbreviation	Value
peta	P	10^{15}
tera	T	10^{12}
giga	G	10^9
mega	M	10^6
kilo	k	10^3
hecto	h	10^2
deca	da	10^1
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}

4. Unit conversions and standard conditions

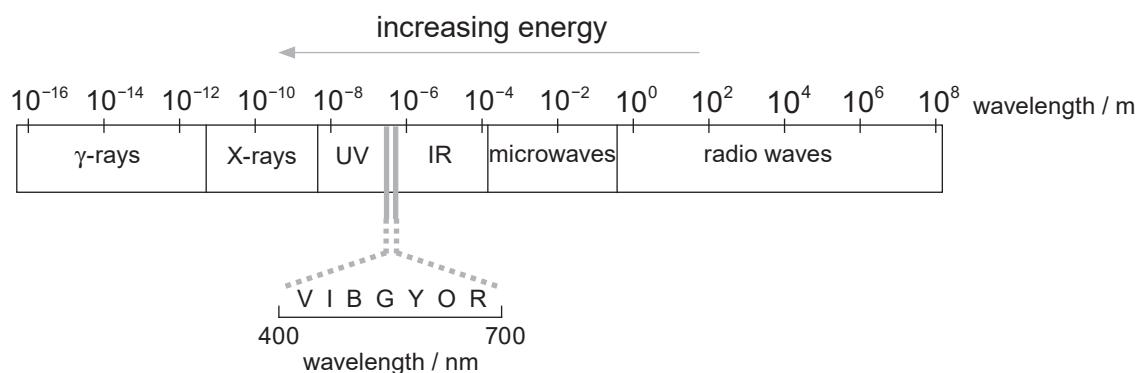
Temperature (K) = temperature ($^{\circ}\text{C}$) + 273.15

$1\text{dm}^3 = 1 \text{ litre} = 1 \times 10^{-3} \text{ m}^3 = 1 \times 10^3 \text{ cm}^3$

STP conditions: 273.15 K and 100 kPa

SATP conditions: 298.15 K and 100 kPa

5. The electromagnetic spectrum



6. Names of the elements

Element	Symbol	Atomic number
actinium	Ac	89
aluminium	Al	13
americium	Am	95
antimony	Sb	51
argon	Ar	18
arsenic	As	33
astatine	At	85
barium	Ba	56
berkelium	Bk	97
beryllium	Be	4
bismuth	Bi	83
bohrium	Bh	107
boron	B	5
bromine	Br	35
cadmium	Cd	48
caesium	Cs	55
calcium	Ca	20
californium	Cf	98
carbon	C	6
cerium	Ce	58
chlorine	Cl	17
chromium	Cr	24
cobalt	Co	27
copernicium	Cn	112
copper	Cu	29
curium	Cm	96
darmstadtium	Ds	110
dubnium	Db	105

Element	Symbol	Atomic number
dysprosium	Dy	66
einsteinium	Es	99
erbium	Er	68
europium	Eu	63
fermium	Fm	100
flerovium	Fl	114
fluorine	F	9
francium	Fr	87
gadolinium	Gd	64
gallium	Ga	31
germanium	Ge	32
gold	Au	79
hafnium	Hf	72
hassium	Hs	108
helium	He	2
holmium	Ho	67
hydrogen	H	1
indium	In	49
iodine	I	53
iridium	Ir	77
iron	Fe	26
krypton	Kr	36
lanthanum	La	57
lawrencium	Lr	103
lead	Pb	82
lithium	Li	3
livermorium	Lv	116
lutetium	Lu	71

Element	Symbol	Atomic number	Element	Symbol	Atomic number
roentgenium	Rg	111	rubidium	Rb	37
ruthenium	Ru	44	rutherfordium	Rf	104
samarium	Sm	62	scandium	Sc	21
seaborgium	Sg	106	selenium	Se	34
silicon	Si	14	silver	Ag	47
neon	Ne	10	sodium	Na	11
neptunium	Np	93	strontium	Sr	38
nickel	Ni	28	sulfur	S	16
nihonium	Nh	113	tantalum	Ta	73
niobium	Nb	41	technetium	Tc	43
nitrogen	N	7	tellurium	Te	52
nobelium	No	102	tennesseine	Ts	117
oganesson	Og	118	terbium	Tb	65
osmium	Os	76	thallium	Tl	81
oxygen	O	8	thorium	Th	90
palladium	Pd	46	thulium	Tm	69
phosphorus	P	15	tin	Sn	50
platinum	Pt	78	titanium	Ti	22
plutonium	Pu	94	tungsten	W	74
polonium	Po	84	uranium	U	92
potassium	K	19	vanadium	V	23
praseodymium	Pr	59	xenon	Xe	54
promethium	Pm	61	ytterbium	Yb	70
protactinium	Pa	91	yttrium	Y	39
radium	Ra	88	zinc	Zn	30
radon	Rn	86	zirconium	Zr	40
rhenium	Re	75			
rhodium	Rh	45			

Element	Symbol	Atomic number	Element	Symbol	Atomic number
magnesium	Mg	12	rhodium	Rh	45
manganese	Mn	25	rubidium	Rb	37
meitnerium	Mt	109	ruthenium	Ru	44
mendelevium	Md	101	rutherfordium	Rf	104
mercury	Hg	80	samarium	Sm	62
molybdenum	Mo	42	scandium	Sc	21
moscovium	Mc	115	seaborgium	Sg	106
neodymium	Nd	60	selenium	Se	34
neon	Ne	10	silicon	Si	14
neptunium	Np	93	silver	Ag	47
nickel	Ni	28	sodium	Na	11
nihonium	Nh	113	strontium	Sr	38
niobium	Nb	41	sulfur	S	16
nitrogen	N	7	tantalum	Ta	73
nobelium	No	102	technetium	Tc	43
oganesson	Og	118	tellurium	Te	52
osmium	Os	76	tennesseine	Ts	117
oxygen	O	8	terbium	Tb	65
palladium	Pd	46	thallium	Tl	81
phosphorus	P	15	thorium	Th	90
platinum	Pt	78	thulium	Tm	69
plutonium	Pu	94	tin	Sn	50
polonium	Po	84	titanium	Ti	22
potassium	K	19	tungsten	W	74
praseodymium	Pr	59	uranium	U	92
promethium	Pm	61	vanadium	V	23
protactinium	Pa	91	xenon	Xe	54
radium	Ra	88	ytterbium	Yb	70
radon	Rn	86	yttrium	Y	39
rhenium	Re	75	zinc	Zn	30
rhodium	Rh	45	zirconium	Zr	40

7. The periodic table

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
	Atomic number																		
	Element																		
	Relative atomic mass																		
1	H 1.01																		
2	Li 6.94	4 Be 9.01																	
3	Na 22.99	Mg 24.31																	
4	K 39.10	Ca 40.08	Sc 44.96	Ti 47.87	V 50.94	Cr 52.00	Mn 54.94	Fe 55.85	Co 58.93	Ni 58.69	Cu 63.55	Zn 65.38	Ga 69.72	Ge 72.63	As 74.92	Se 78.96	Br 79.90	Kr 83.80	
5	Rb 85.47	Sr 87.62	Y 88.91	Zr 91.22	Nb 92.91	Tc 95.96	Mo (98)	Ru 101.07	Rh 102.91	Pd 106.42	Ag 107.87	Cd 112.41	In 114.82	Sn 118.71	Sb 121.76	Te 127.60	I 131.29	Xe (222)	
6	Cs 132.91	Ba 137.33	La 138.91	Hf 178.49	Ta 180.95	W 183.84	Re 186.21	Os 190.23	Ir 192.22	Pt 195.08	Au 196.97	Hg 200.59	Tl 204.38	Pb 207.20	Bi 208.98	Po (209)	At (210)	Rn (222)	
7	Fr (223)	Ra (226)	Ac (227)	Rf (267)	Db (268)	Sg (269)	Bh (270)	Hs (269)	Mt (278)	108 (269)	109 (270)	Ds (281)	110 (269)	Rg (281)	Cn (285)	Nh (286)	Fm (289)	Ts (293)	Og (294)
†	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05	71 Lu 174.97					
‡	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)					

8. Melting points and boiling points of the elements at 101.325 kPa

	Element		Melting point / °C	Boiling point / °C	
H -259.2					He -268.9
Li 180.5 1342	B 1287 Be 2468	C 4000	-2077 3500	-210.0 -195.8	N -183.0
Na 97.79 882.9	D 650.0 Mg 1090	E 660.3	-1414 115.2	-218.8 -183.0	O -188.1
K 758.8	F 842.0 Ca 1484	G 2519	44.15 115.2	-219.7 -101.5	F -248.6
Rb 687.8	H 768.8 Sr 1377	I 3265	444.6 280.5	-189.3 -34.04	Ne -246.0
Cs 670.8	J 725.0 Ba 1845	K 2519	280.5	-185.8	Ar
Fr 676.8	L 27.00 Ra 1140	M 3265			
	N 1050 Ac † 3200				

T	795 3433	935 3510	1024 3074	1042 (2730)	826 1791	1313 1596	1360 3273	1410 3230	1472 2567	1529 2694	1545 2900	824 1950	1663 1194	Lu 3402
#	1750 4788	1572 (4000)	1135 3818	637 (3900)	640 3230	1176 1340 (2067)	1340 Cm 3110	986 Bk (2623)	900 (860) Ef	900 Fm	827 Md	No	Lr	



9. First ionization energy, electron affinity and electronegativity of the elements

		First ionization energy / kJ mol ⁻¹		Electron affinity (EA) / kJ mol ⁻¹ (2nd EA / kJ mol ⁻¹)			
		Element					
		Electronegativity					
H	-73 2.2						
Li	-60 1.0	Be 1.6					
Mg	-53 0.9	Mg 1.3					
K	-48 0.8	Ca 1.0	Sc 1.4	Ti 1.5	V 1.6		
Rb	-47 0.8	Sr 1.0	Y 1.2	Zr 1.3	Nb 1.6		
Cs	-46 0.8	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5		
Fr	-47 0.7	Ra 0.9		Ac 1.1	Ac # 1.1		

		First ionization energy / kJ mol ⁻¹		Electron affinity (EA) / kJ mol ⁻¹ (2nd EA / kJ mol ⁻¹)			
		Element					
		Electronegativity					
H	-73 2.2						
Li	-900 1.0	Be 1.6					
Mg	-738 0.9	Mg 1.3					
K	-590 1.0	Ca 1.4	Sc 1.5	Ti 1.6	V 1.7		
Rb	-600 1.0	Sr 1.2	Y 1.3	Zr 1.3	Nb 1.6		
Cs	-503 0.9	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5		
Fr	-509 0.7	Ra 0.9		Ac 1.1	Ac # 1.1		
Ce	-63 1.1	Pr 1.1	Nd 1.1	Pm 1.1	Pm		
Th	-528 1.3	Pa 1.5	U 1.7	Np 1.3	Np		
Tb	-93 598	Eu 605	Sm 581	Gd 576	Gd 578		
Am	-185 605	Eu 581	Sm 576	Tb 578	Tb 593		
Cm	-185 605	Am 581	Eu 576	Dy 606	Dy 566		
Bk	-185 605	Cm 581	Am 576	Cf 598	Cf 573		
Fm	-185 605	Bk 581	Cm 576	Es 619	Es 581		
Md	-185 605	Fm 598	Bk 578	Er 627	Er 589		
No	-185 605	Md 619	Fm 619	Tm 635	Tm 597		
Lr	-185 605	No 627	Md 635	Yb 642	Yb 599		
Lu	-34 2.2	Lr 642	No 635	At 473	At 603		

		First ionization energy / kJ mol ⁻¹		Electron affinity (EA) / kJ mol ⁻¹ (2nd EA / kJ mol ⁻¹)			
		Element					
		Electronegativity					
He	-27 2.0	B 2.0	C 2.6	N 3.0	O 3.4		
Al	-42 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2		
Ge	-787 1.8	Ge 2.0	As 2.2	Se 2.6	Br 3.0		
In	-134 1.8	In 2.0	Sn 2.0	Te 2.1	I 2.7		
Ga	-119 1.8	Ga 1.8	Sn 1.8	Te 2.1	Xe 2.7		
Tl	-78 1.8	Tl 1.8	Pb 1.8	Bi 1.9	Rn 2.2		
Ho	-141 1.2	Ho 1.2	Er 1.2	Tm 1.3	Lu 1.0		

10. Atomic and ionic radii of the elements

The values for atomic radii used in this table are the covalent radii of the elements.

32 H	130 Li 76 (1+)	99 Be 45 (2+)	160 Na 102 (1+)	140 Mg 72 (2+)	Element	Atomic radius / 10 ⁻¹² m	Ionic radius / 10 ⁻¹² m (charge)
200 K 138 (1+)	174 Ca 100 (2+)	159 Sc 75 (3+)	148 Ti 61 (4+)	144 V 54 (5+)	130 Cr 44 (6+)	129 Mn 53 (4+)	124 Fe 55 (3+)
215 Rb 152 (1+)	190 Sr 118 (2+)	176 Y 90 (3+)	164 Zr 72 (4+)	156 Nb 64 (5+)	146 Tc 65 (4+)	138 Mo 62 (4+)	136 Ru 62 (4+)
238 Cs 167 (1+)	206 Ba 135 (2+)	194 La 103 (3+)	164 Hf 71 (4+)	158 Ta 64 (5+)	150 W 64 (5+)	141 Re 60 (6+)	136 Os 53 (7+)
242 Fr	211 Ra		201 Ac ‡				

†	184 Ce 101 (3+) 87 (4+)	190 Pr 99 (3+) 85 (4+)	188 Nd 98 (3+)	186 Pm 97 (3+)	185 Sm 96 (3+)	183 Eu 95 (3+)	182 Gd 94 (3+)	181 Tb 92 (3+) 76 (4+)	180 Dy 91 (3+)	179 Ho 90 (3+)	177 Er 89 (3+)	178 Tm 88 (3+)	174 Yb 87 (3+)	178 Lu 86 (3+)
‡	190 Th 94 (4+)	184 Pa 104 (3+) 90 (4+)	183 U 89 (4+) 73 (6+)	180 Np 101 (3+) 87 (4+)	180 Pu 100 (3+) 86 (4+)	173 Am 98 (3+) 85 (4+)	168 Cm 97 (3+)	168 Bk 96 (3+)	165 Es 95 (3+)	167 Fm	173 Md	176 No 110 (2+)	161 Lr	

11. Covalent or average covalent bond lengths

Single bonds

Bond	Length / 10^{-12} m	Bond	Length / 10^{-12} m	Bond	Length / 10^{-12} m	Bond	Length / 10^{-12} m
H — H	74	N — H	101	Si — H	148	S — H	134
H — F	92	N — N	146	Si — Si	232	S — S	205
H — Cl	128	N — O	136	Si — S	215	S — F	158
H — Br	141	N — Si	174	Si — F	156	S — Cl	199
H — I	160	N — S	175	Si — Cl	202	S — Br	227
		N — F	136	Si — Br	216		
C — H	108	N — Cl	197	Si — I	243	F — F	142
C — C	154	N — Br	214			F — Cl	163
C — N	147			P — H	142	F — Br	176
C — O	143	O — H	97	P — P	221	F — I	191
C — Si	185	O — O	148	P — S	210		
C — P	184	O — Si	163	P — F	154	Cl — Cl	199
C — S	182	O — P	154	P — Cl	203	Cl — Br	214
C — F	138	O — S	161	P — Br	220	Cl — I	232
C — Cl	177	O — F	142	P — I	247		
C — Br	194	O — Cl	170			Br — Br	228
C — I	214					Br — I	247
						I — I	267

Multiple bonds

Bond	Length / 10^{-12} m	Bond	Length / 10^{-12} m	Bond	Length / 10^{-12} m
C = C	134	N = N	125	O = O	121
C = N	130	N = O	114	O = S	143
C = O	122				
C = S	156			S = S	189
C ≡ C	120	N ≡ N	110		
C ≡ N	116				
C ≡ O	113				

12. Bond enthalpies or average bond enthalpies at 298.15 K

Single bonds

Bond	Enthalpy / kJ mol ⁻¹	Bond	Enthalpy / kJ mol ⁻¹	Bond	Enthalpy / kJ mol ⁻¹	Bond	Enthalpy / kJ mol ⁻¹
H — H	436	N — H	391	Si — H	323	S — H	364
H — F	567	N — N	158	Si — Si	226	S — S	266
H — Cl	431	N — O	214	Si — S	293	S — F	327
H — Br	366	N — F	278	Si — F	597	S — Cl	271
H — I	298	N — Cl	192	Si — Cl	400	S — Br	218
				Si — Br	330		
C — H	414	O — H	463	Si — I	234	F — F	159
C — C	346	O — O	144			F — Cl	255
C — N	286	O — Si	466	P — H	322	F — Br	249
C — O	358	O — P	363	P — P	198	F — I	280
C — Si	307	O — F	191	P — F	490		
C — P	264	O — Cl	206	P — Cl	322	Cl — Cl	242
C — S	289	O — Br	201	P — Br	264	Cl — Br	219
C — F	492	O — I	201	P — I	184	Cl — I	211
C — Cl	324						
C — Br	285					Br — Br	193
C — I	228					Br — I	178
						I — I	151

Multiple bonds

Bond	Enthalpy / kJ mol ⁻¹	Bond	Enthalpy / kJ mol ⁻¹	Bond	Enthalpy / kJ mol ⁻¹
C = C	614	N = N	470	O = O	498
C = N	615	N = O	587	O = S	522
C = O	804				
C = S	536			S = S	429
C ≡ C	839	N ≡ N	945		
C ≡ N	890				
C ≡ O	1077				

13. Thermodynamic data (selected compounds)

Substance	Formula	State	$\Delta H_f^\ominus / \text{kJ mol}^{-1}$	$\Delta G_f^\ominus / \text{kJ mol}^{-1}$	$S^\ominus / \text{J K}^{-1} \text{ mol}^{-1}$
methane	CH ₄	g	-74	-50	+186
ethane	C ₂ H ₆	g	-84	-32	+230
propane	C ₃ H ₈	g	-105	-24	+270
butane	C ₄ H ₁₀	g	-126	-17	+310
pentane	C ₅ H ₁₂	l	-173		
hexane	C ₆ H ₁₄	l	-199		
ethene	C ₂ H ₄	g	+52	+68	+220
propene	C ₃ H ₆	g	+20	+62	+267
but-1-ene	C ₄ H ₈	g	+0.1	+71	+306
cis-but-2-ene	C ₄ H ₈	g	-7	+66	+301
trans-but-2-ene	C ₄ H ₈	g	-11	+63	+297
ethyne	C ₂ H ₂	g	+228	+211	+201
propyne	C ₃ H ₄	g	+185	+194	+248
buta-1,3-diene	C ₄ H ₆	g	+110	+151	+279
cyclohexane	C ₆ H ₁₂	l	-156		
benzene	C ₆ H ₆	l	+49	+125	+173
methylbenzene	C ₆ H ₅ CH ₃	l	+12		
ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	l	-12		
phenylethene	C ₆ H ₅ CHCH ₂	l	+104		
chloromethane	CH ₃ Cl	g	-82	-58	+235
dichloromethane	CH ₂ Cl ₂	l	-124		+178
trichloromethane	CHCl ₃	l	-134	-74	+202
bromomethane	CH ₃ Br	g	-36	-26	+246
iodomethane	CH ₃ I	l	-14		+163
chloroethane	C ₂ H ₅ Cl	g	-137	-53	
bromoethane	C ₂ H ₅ Br	l	-90	-26	+199
chlorobenzene	C ₆ H ₅ Cl	l	+11		
methanol	CH ₃ OH	l	-239	-167	+127
ethanol	C ₂ H ₅ OH	l	-278	-175	+161
phenol	C ₆ H ₅ OH	s	-165		+144
methanal	HCHO	g	-109	-102	+219
ethanal	CH ₃ CHO	g	-166	-133	+264
propanone	(CH ₃) ₂ CO	l	-248		+200
methanoic acid	HCOOH	l	-425	-361	+129
ethanoic acid	CH ₃ COOH	l	-484	-390	+160
benzoic acid	C ₆ H ₅ COOH	s	-385		+168
methylamine	CH ₃ NH ₂	g	-23	+32	+243
water	H ₂ O	l	-286	-237	+70
steam	H ₂ O	g	-242	-229	+189
carbon monoxide	CO	g	-111	-137	+198
carbon dioxide	CO ₂	g	-394	-394	+214
hydrogen bromide	HBr	g	-36	-53	+199
hydrogen chloride	HCl	g	-92	-95	+187
hydrogen fluoride	HF	g	-273	-275	+174
hydrogen iodide	HI	g	+26	+2	+207

14. Enthalpies of combustion

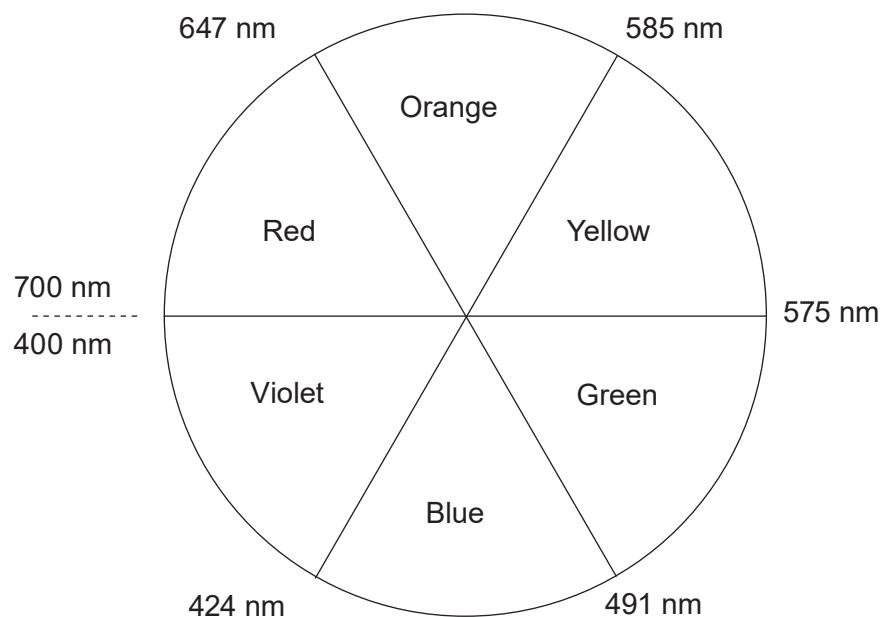
The values of the molar enthalpy of combustion (ΔH_c^\ominus) in the following table refer to a temperature of 298.15 K and a pressure of 100 kPa.

Substance	Formula	State	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$
hydrogen	H ₂	g	-286
sulfur	S	s	-297
carbon (graphite)	C	s	-394
carbon monoxide	CO	g	-283
methane	CH ₄	g	-891
ethane	C ₂ H ₆	g	-1561
propane	C ₃ H ₈	g	-2219
butane	C ₄ H ₁₀	g	-2878
pentane	C ₅ H ₁₂	l	-3509
hexane	C ₆ H ₁₄	l	-4163
octane	C ₈ H ₁₈	l	-5470
cyclohexane	C ₆ H ₁₂	l	-3920
ethene	C ₂ H ₄	g	-1411
buta-1,3-diene	C ₄ H ₆	g	-2541
ethyne	C ₂ H ₂	g	-1301
benzene	C ₆ H ₆	l	-3268
methylbenzene	C ₆ H ₅ CH ₃	l	-3910
naphthalene	C ₁₀ H ₈	s	-5156
chloroethane	C ₂ H ₅ Cl	g	-1413
iodoethane	C ₂ H ₅ I	l	-1463
trichloromethane	CHCl ₃	l	-473
methanol	CH ₃ OH	l	-726
ethanol	C ₂ H ₅ OH	l	-1367

Substance	Formula	State	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$
propan-1-ol	C ₃ H ₇ OH	l	-2021
butan-1-ol	C ₄ H ₉ OH	l	-2676
cyclohexanol	C ₆ H ₁₁ OH	s	-3728
phenol	C ₆ H ₅ OH	s	-3053
ethoxyethane	(C ₂ H ₅) ₂ O	l	-2724
methanal	HCHO	g	-571
ethanal	CH ₃ CHO	g	-1167
benzaldehyde	C ₆ H ₅ CHO	l	-3525
propanone	(CH ₃) ₂ CO	l	-1790
pentan-3-one	(C ₂ H ₅) ₂ CO	l	-3100
phenylethanol	CH ₃ COC ₆ H ₅	l	-4149
methanoic acid	HCOOH	l	-255
ethanoic acid	CH ₃ COOH	l	-874
benzoic acid	C ₆ H ₅ COOH	s	-3228
ethanedioic acid	(COOH) ₂	s	-243
ethyl ethanoate	CH ₃ COOC ₂ H ₅	l	-2238
ethanamide	CH ₃ CONH ₂	s	-1186
methylamine	CH ₃ NH ₂	g	-1086
phenylamine	C ₆ H ₅ NH ₂	l	-3393
nitrobenzene	C ₆ H ₅ NO ₂	l	-3088
urea	CO(NH ₂) ₂	s	-633
glucose	C ₆ H ₁₂ O ₆	s	-2803
sucrose	C ₁₂ H ₂₂ O ₁₁	s	-5640



15. Colour wheel with wavelengths of the visible spectrum



16. Lattice enthalpies at 298.15 K (experimental values)

The lattice enthalpy values ($\Delta H_{\text{lattice}}^{\ominus}$) in the following tables relate to the endothermic process $M_aX_b(s) \rightarrow aM^{b+}(g) + bX^{a-}(g)$ in which the gaseous ions of a crystal are separated to an infinite distance from each other.

The data in these tables are experimental values obtained by means of a suitable Born–Haber cycle.

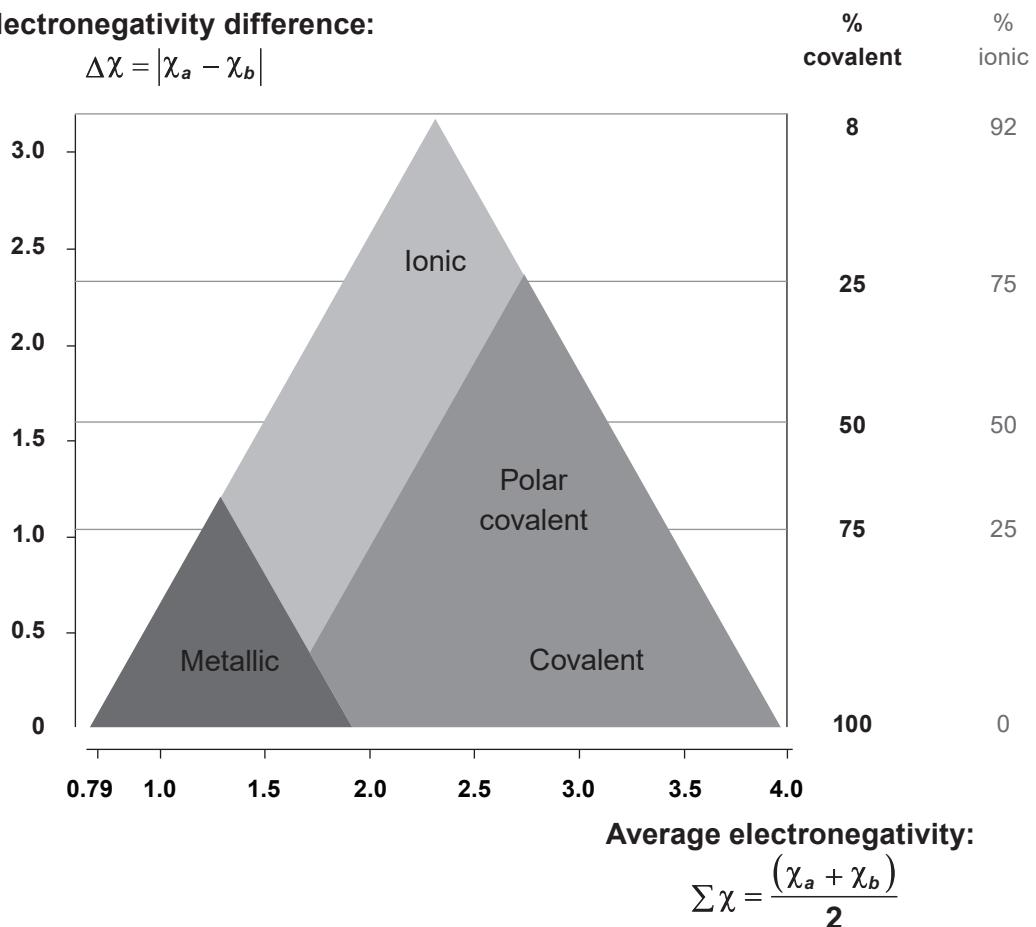
Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$			
	F	Cl	Br	I
Li	1049	864	820	764
Na	930	790	754	705
K	829	720	691	650
Rb	795	695	668	632
Cs	759	670	647	613

Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$	Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$
CaF ₂	2651	SrO	3223
BeCl ₂	3033	BaO	3054
MgCl ₂	2540	CuCl ₂	2824
CaCl ₂	2271	AgF	974
SrCl ₂	2170	AgCl	918
BaCl ₂	2069	AgBr	905
MgO	3791	AgI	892
CaO	3401		

17. Triangular bonding diagram (van Arkel–Ketelaar triangle)

Electronegativity difference:

$$\Delta\chi = |\chi_a - \chi_b|$$



18. Acid–base indicators

Indicator	pK_a	pH range	Colour change	
			Acid	Alkali
methyl orange	3.7	3.1–4.4	red	yellow
bromophenol blue	4.2	3.0–4.6	yellow	blue
bromocresol green	4.7	4.0–5.6	yellow	blue
methyl red	5.1	4.4–6.2	red	yellow
bromothymol blue	7.0	6.0–7.6	yellow	blue
phenol red	7.9	6.4–8.0	yellow	red
phenolphthalein	9.6	8.0–10.0	colourless	pink

19. Standard reduction potentials at 298.15 K

Oxidized species	Reduced species	E^\ominus / V
$\text{Li}^+(\text{aq}) + \text{e}^- \rightleftharpoons \text{Li(s)}$		-3.04
$\text{K}^+(\text{aq}) + \text{e}^- \rightleftharpoons \text{K(s)}$		-2.93
$\text{Ca}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Ca(s)}$		-2.87
$\text{Na}^+(\text{aq}) + \text{e}^- \rightleftharpoons \text{Na(s)}$		-2.71
$\text{Mg}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Mg(s)}$		-2.37
$\text{Al}^{3+}(\text{aq}) + 3\text{e}^- \rightleftharpoons \text{Al(s)}$		-1.66
$\text{Mn}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Mn(s)}$		-1.18
$\text{H}_2\text{O(l)} + \text{e}^- \rightleftharpoons \frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$		-0.83
$\text{Zn}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Zn(s)}$		-0.76
$\text{Fe}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Fe(s)}$		-0.45
$\text{Ni}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Ni(s)}$		-0.26
$\text{Sn}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Sn(s)}$		-0.14
$\text{Pb}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Pb(s)}$		-0.13
$\text{H}^+(\text{aq}) + \text{e}^- \rightleftharpoons \frac{1}{2}\text{H}_2(\text{g})$		0.00
$\text{Cu}^{2+}(\text{aq}) + \text{e}^- \rightleftharpoons \text{Cu}^+(\text{aq})$		+0.15
$\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O(l)}$		+0.17
$\text{Cu}^{2+}(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{Cu(s)}$		+0.34
$\frac{1}{2}\text{O}_2(\text{g}) + \text{H}_2\text{O(l)} + 2\text{e}^- \rightleftharpoons 2\text{OH}^-(\text{aq})$		+0.40
$\text{Cu}^+(\text{aq}) + \text{e}^- \rightleftharpoons \text{Cu(s)}$		+0.52
$\frac{1}{2}\text{I}_2(\text{s}) + \text{e}^- \rightleftharpoons \text{I}^-(\text{aq})$		+0.54
$\text{Fe}^{3+}(\text{aq}) + \text{e}^- \rightleftharpoons \text{Fe}^{2+}(\text{aq})$		+0.77
$\text{Ag}^+(\text{aq}) + \text{e}^- \rightleftharpoons \text{Ag(s)}$		+0.80
$\frac{1}{2}\text{Br}_2(\text{l}) + \text{e}^- \rightleftharpoons \text{Br}^-(\text{aq})$		+1.09
$\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^- \rightleftharpoons \text{H}_2\text{O(l)}$		+1.23
$\text{Cr}_2\text{O}_7^{2-}(\text{aq}) + 14\text{H}^+(\text{aq}) + 6\text{e}^- \rightleftharpoons 2\text{Cr}^{3+}(\text{aq}) + 7\text{H}_2\text{O(l)}$		+1.36
$\frac{1}{2}\text{Cl}_2(\text{g}) + \text{e}^- \rightleftharpoons \text{Cl}^-(\text{aq})$		+1.36
$\text{MnO}_4^-(\text{aq}) + 8\text{H}^+(\text{aq}) + 5\text{e}^- \rightleftharpoons \text{Mn}^{2+}(\text{aq}) + 4\text{H}_2\text{O(l)}$		+1.51
$\frac{1}{2}\text{F}_2(\text{g}) + \text{e}^- \rightleftharpoons \text{F}^-(\text{aq})$		+2.87

20. Infrared data

Characteristic ranges for infrared absorption due to stretching vibrations in organic molecules

Bond	Types of organic molecules	Wavenumber / cm ⁻¹	Intensity
C—I	iodoalkanes	490–620	strong
C—Br	bromoalkanes	500–600	strong
C—Cl	chloroalkanes	600–800	strong
C—F	fluoroalkanes	1000–1400	strong
C—O	alcohols, esters, ethers	1050–1410	strong
C=C	alkenes	1620–1680	medium-weak; multiple bands
C=O	aldehydes, ketones, carboxylic acids and esters	1700–1750	strong
C≡C	alkynes	2100–2260	variable
O—H	carboxylic acids (with hydrogen bonding)	2500–3000	strong, very broad
C—H	alkanes, alkenes, arenes	2850–3090	strong
O—H	alcohols and phenols (with hydrogen bonding)	3200–3600	strong, broad
N—H	primary amines	3300–3500	medium; two bands



21. ^1H NMR data

Typical proton chemical shift values (δ) relative to tetramethylsilane (TMS)

R represents an alkyl group, and Hal represents F, Cl, Br or I.

These values may vary for different solvents and conditions.

Type of proton	Chemical shift / ppm
$-\text{CH}_3$	0.9–1.0
$-\text{CH}_2-\text{R}$	1.3–1.4
$-\text{CHR}_2$	1.5
	2.0–2.5
	2.2–2.7
	2.5–3.5
$-\text{C}\equiv\text{C}-\text{H}$	1.8–3.1
$-\text{CH}_2-\text{Hal}$	3.5–4.4
$\text{R}-\text{O}-\text{CH}_2-$	3.3–3.7
	3.7–4.8
	9.0–13.0
$\text{R}-\text{O}-\text{H}$	1.0–6.0
$-\text{CH}=\text{CH}_2$	4.5–6.0
	4.0–12.0
	6.9–9.0
	9.4–10.0

22. Mass spectral fragments lost

Mass lost (M_r)	Possible neutral fragment lost
15	$\bullet\text{CH}_3$
17	$\bullet\text{OH}$
18	H_2O
28	$\text{CH}_2=\text{CH}_2$ CO
29	$\bullet\text{CH}_2\text{CH}_3$ $\bullet\text{CHO}$
31	$\bullet\text{OCH}_3$
45	$\bullet\text{COOH}$

23. Uncertainties

If: $y = a \pm b$	then: $\Delta y = \Delta a + \Delta b$
If: $y = \frac{ab}{c}$	then: $\frac{\Delta y}{y} = \frac{\Delta a}{a} + \frac{\Delta b}{b} + \frac{\Delta c}{c}$
If: $y = a^n$	then: $\frac{\Delta y}{y} = \left n \frac{\Delta a}{a} \right $

24. References

Data in sections 7, 8, 9, 10, 11, 12, 13, 14, 16, 18, 19, 20, 21 and 22 were taken fully or in part from:

Blackman, A., Gahan, L. R., Aylward, G. H., & Findlay, T. J. V. (2014). *Aylward and Findlay's SI Chemical Data*. (7th ed.). John Wiley & Sons.

National Institute of Standards and Technology. (2021). *NIST Chemistry WebBook SRD 69, NIST Standard Reference Database*. U.S. Department of Commerce. <http://webbook.nist.gov>

Rumble, J. R. (Ed.). (2019). *CRC Handbook of Chemistry and Physics*. (100th ed.). CRC Press.

Data in section 17 are reproduced with permission from the author:

Leach, M. R. (2021). *The Chemogenesis Web Book: Timeline of structural theory*. http://www.metasynthesis.com/webbook/30_timeline/timeline.html

Updates to the publication

This section outlines the updates made to this publication over the past two years. The changes are ordered from the most recent to the oldest updates. Minor spelling and typographical corrections are not listed.

Changes for February 2024

11. Covalent or average covalent bond lengths

The bond length for F — I was corrected to 191×10^{-12} m.

18. Acid–base indicators

The pH ranges for bromocresol green, phenol red and phenolphthalein were updated according to the latest published data.

23. Uncertainties

This section listing uncertainties propagation formulae was added.