

# Chemistry data booklet

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

Version 1.1

# Diploma Programme

## Chemistry data booklet

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

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## 2. Physical constants

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

---

### 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	$\mu$	$10^{-6}$
nano	n	$10^{-9}$
pico	p	$10^{-12}$
femto	f	$10^{-15}$

---

## 4. Unit conversions and standard conditions

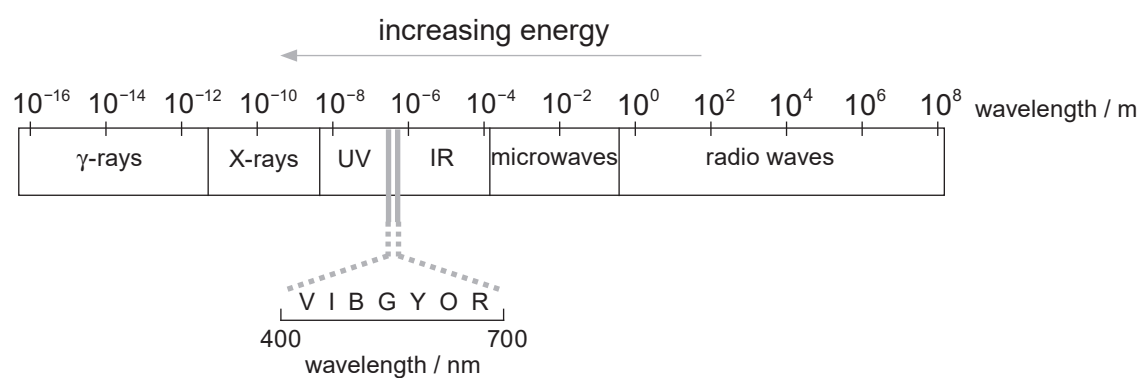
Temperature (K) = temperature (°C) + 273.15

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

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
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
magnesium	Mg	12
manganese	Mn	25
meitnerium	Mt	109
mendelevium	Md	101
mercury	Hg	80
molybdenum	Mo	42
moscovium	Mc	115
neodymium	Nd	60
neon	Ne	10
neptunium	Np	93
nickel	Ni	28
nihonium	Nh	113
niobium	Nb	41
nitrogen	N	7
nobelium	No	102
oganesson	Og	118
osmium	Os	76
oxygen	O	8
palladium	Pd	46
phosphorus	P	15
platinum	Pt	78
plutonium	Pu	94
polonium	Po	84
potassium	K	19
praseodymium	Pr	59
promethium	Pm	61
protactinium	Pa	91
radium	Ra	88
radon	Rn	86
rhenium	Re	75
rhodium	Rh	45

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
sodium	Na	11
strontium	Sr	38
sulfur	S	16
tantalum	Ta	73
technetium	Tc	43
tellurium	Te	52
tennessine	Ts	117
terbium	Tb	65
thallium	Tl	81
thorium	Th	90
thulium	Tm	69
tin	Sn	50
titanium	Ti	22
tungsten	W	74
uranium	U	92
vanadium	V	23
xenon	Xe	54
ytterbium	Yb	70
yttrium	Y	39
zinc	Zn	30
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
1	1 <b>H</b> 1.01																	2 <b>He</b> 4.00
2	3 <b>Li</b> 6.94	4 <b>Be</b> 9.01														8 <b>O</b> 16.00	9 <b>F</b> 19.00	10 <b>Ne</b> 20.18
3	11 <b>Na</b> 22.99	12 <b>Mg</b> 24.31														16 <b>S</b> 32.07	17 <b>Cl</b> 35.45	18 <b>Ar</b> 39.95
4	19 <b>K</b> 39.10	20 <b>Ca</b> 40.08	21 <b>Sc</b> 44.96	22 <b>Ti</b> 47.87	23 <b>V</b> 50.94	24 <b>Cr</b> 52.00	25 <b>Mn</b> 54.94	26 <b>Fe</b> 55.85	27 <b>Co</b> 58.93	28 <b>Ni</b> 58.69	29 <b>Cu</b> 63.55	30 <b>Zn</b> 65.38	31 <b>Ga</b> 69.72	32 <b>Ge</b> 72.63	33 <b>As</b> 74.92	34 <b>Se</b> 78.96	35 <b>Br</b> 79.90	36 <b>Kr</b> 83.80
5	37 <b>Rb</b> 85.47	38 <b>Sr</b> 87.62	39 <b>Y</b> 88.91	40 <b>Zr</b> 91.22	41 <b>Nb</b> 92.91	42 <b>Mo</b> 95.96	43 <b>Tc</b> (98)	44 <b>Ru</b> 101.07	45 <b>Rh</b> 102.91	46 <b>Pd</b> 106.42	47 <b>Ag</b> 107.87	48 <b>Cd</b> 112.41	49 <b>In</b> 114.82	50 <b>Sn</b> 118.71	51 <b>Sb</b> 121.76	52 <b>Te</b> 127.60	53 <b>I</b> 126.90	54 <b>Xe</b> 131.29
6	55 <b>Cs</b> 132.91	56 <b>Ba</b> 137.33	57 <b>La †</b> 138.91	72 <b>Hf</b> 178.49	73 <b>Ta</b> 180.95	74 <b>W</b> 183.84	75 <b>Re</b> 186.21	76 <b>Os</b> 190.23	77 <b>Ir</b> 192.22	78 <b>Pt</b> 195.08	79 <b>Au</b> 196.97	80 <b>Hg</b> 200.59	81 <b>Tl</b> 204.38	82 <b>Pb</b> 207.20	83 <b>Bi</b> 208.98	84 <b>Po</b> (209)	85 <b>At</b> (210)	86 <b>Rn</b> (222)
7	87 <b>Fr</b> (223)	88 <b>Ra</b> (226)	89 <b>Ac ‡</b> (227)	104 <b>Rf</b> (267)	105 <b>Db</b> (268)	106 <b>Sg</b> (269)	107 <b>Bh</b> (270)	108 <b>Hs</b> (269)	109 <b>Mt</b> (278)	110 <b>Ds</b> (281)	111 <b>Rg</b> (281)	112 <b>Cn</b> (285)	113 <b>Nh</b> (286)	114 <b>Fl</b> (289)	115 <b>Mc</b> (288)	116 <b>Lv</b> (293)	117 <b>Ts</b> (294)	118 <b>Og</b> (294)
			†															
			‡															
				58 <b>Ce</b> 140.12	59 <b>Pr</b> 140.91	60 <b>Nd</b> 144.24	61 <b>Pm</b> (145)	62 <b>Sm</b> 150.36	63 <b>Eu</b> 151.96	64 <b>Gd</b> 157.25	65 <b>Tb</b> 158.93	66 <b>Dy</b> 162.50	67 <b>Ho</b> 164.93	68 <b>Er</b> 167.26	69 <b>Tm</b> 168.93	70 <b>Yb</b> 173.05	71 <b>Lu</b> 174.97	
				90 <b>Th</b> 232.04	91 <b>Pa</b> 231.04	92 <b>U</b> 238.03	93 <b>Np</b> (237)	94 <b>Pu</b> (244)	95 <b>Am</b> (243)	96 <b>Cm</b> (247)	97 <b>Bk</b> (247)	98 <b>Cf</b> (251)	99 <b>Es</b> (252)	100 <b>Fm</b> (257)	101 <b>Md</b> (258)	102 <b>No</b> (259)	103 <b>Lr</b> (262)	



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

First ionization energy / kJ mol <sup>-1</sup>		Electron affinity (EA) / kJ mol <sup>-1</sup> (2nd EA / kJ mol <sup>-1</sup> )		Electronegativity		Element	
1312	-73						2372
<b>H</b>	2.2						<b>He</b>
520	-60	900					
<b>Li</b>	1.0	<b>Be</b>	1.6				
496	-53	738					
<b>Na</b>	0.9	<b>Mg</b>	1.3				
419	-48	590	-2	633	-18	659	
<b>K</b>	0.8	<b>Ca</b>	1.0	<b>Sc</b>	1.4	<b>Ti</b>	1.5
403	-47	549	-5	600	-30	640	
<b>Rb</b>	0.8	<b>Sr</b>	1.0	<b>Y</b>	1.2	<b>Zr</b>	1.3
376	-46	503	-14	538	-45	659	
<b>Cs</b>	0.8	<b>Ba</b>	0.9	<b>La †</b>	1.1	<b>Hf</b>	1.3
393	-47	509	-10	499	-34		
<b>Fr</b>	0.7	<b>Ra</b>	0.9	<b>Ac ‡</b>	1.1		
801	-27	1086	-122	1402			
<b>B</b>	2.0	<b>C</b>	2.6	<b>N</b>	3.0		
578	-42	787	-134	1012	-72	1000	
<b>Al</b>	1.6	<b>Si</b>	1.9	<b>P</b>	2.2	<b>S</b>	2.6
1314	-141	1681	-328	2081			
<b>O</b>	3.4	<b>F</b>	4.0				
1251	-200	1251	-349	1520			
<b>S</b>	2.6	<b>Cl</b>	3.2				
579	-41	762	-119	944	-78	941	
<b>Ga</b>	1.8	<b>Ge</b>	2.0	<b>As</b>	2.2	<b>Se</b>	2.6
558	-29	709	-107	831	-101	869	
<b>In</b>	1.8	<b>Sn</b>	2.0	<b>Sb</b>	2.0	<b>Te</b>	2.1
589	-36	716	-35	703	-91	812	
<b>Tl</b>	1.8	<b>Pb</b>	1.8	<b>Bi</b>	1.9	<b>Po</b>	2.0
566	-112	573	< 0	581			
<b>Dy</b>	1.2	<b>Ho</b>	1.2				
547	-83	593					
<b>Eu</b>	1.2	<b>Gd</b>	1.2				
545							
<b>Sm</b>	1.2	<b>Pm</b>					
534	-63	528	-93	533	-185	539	
<b>Ce</b>	1.1	<b>Pr</b>	1.1	<b>Nd</b>	1.1		
609	568	598	605	581	576	578	
<b>Th</b>	1.3	<b>Pa</b>	1.5	<b>U</b>	1.7		
566	-112	573	606	619			
<b>Tb</b>	1.2	<b>Cf</b>		<b>Es</b>			
589	-99	603	597	627	635	642	
<b>Er</b>	1.2	<b>Tm</b>	1.3	<b>Md</b>			
581							
<b>Ho</b>	1.2	<b>Yb</b>	1.3	<b>No</b>			
581							
<b>Dy</b>	1.2	<b>Lu</b>	1.0				
581							
<b>Er</b>	1.2	<b>Yb</b>	1.3				
581							
<b>Ho</b>	1.2	<b>Lu</b>	1.0				

†	534	-63	528	-93	533	-185	539	545	547	-83	593	566	-112	573	< 0	581	589	-99	603	2	524	-33						
	<b>Ce</b>	1.1	<b>Pr</b>	1.1	<b>Nd</b>	1.1	<b>Pm</b>	<b>Sm</b>	<b>Eu</b>	1.2	<b>Gd</b>	1.2	<b>Tb</b>	1.2	<b>Dy</b>	1.2	<b>Ho</b>	1.2	<b>Er</b>	1.2	<b>Tm</b>	1.3	<b>Yb</b>	1.3	<b>Lu</b>	1.0		
‡	609	568	598	605	581	576	578	598	598	606	619	627	635	642	473													
	<b>Th</b>	1.3	<b>Pa</b>	1.5	<b>U</b>	1.7	<b>Np</b>	1.3	<b>Pu</b>	1.3	<b>Am</b>	1.3	<b>Cm</b>	1.3	<b>Bk</b>	1.3	<b>Cf</b>	1.3	<b>Es</b>	1.3	<b>Fm</b>	1.3	<b>Md</b>	1.3	<b>No</b>	1.3	<b>Lr</b>	1.3



## 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 $\equiv$ C	120	N $\equiv$ N	110		
C $\equiv$ N	116				
C $\equiv$ O	113				

## 12. Bond enthalpies or average bond enthalpies at 298.15 K

### Single bonds

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

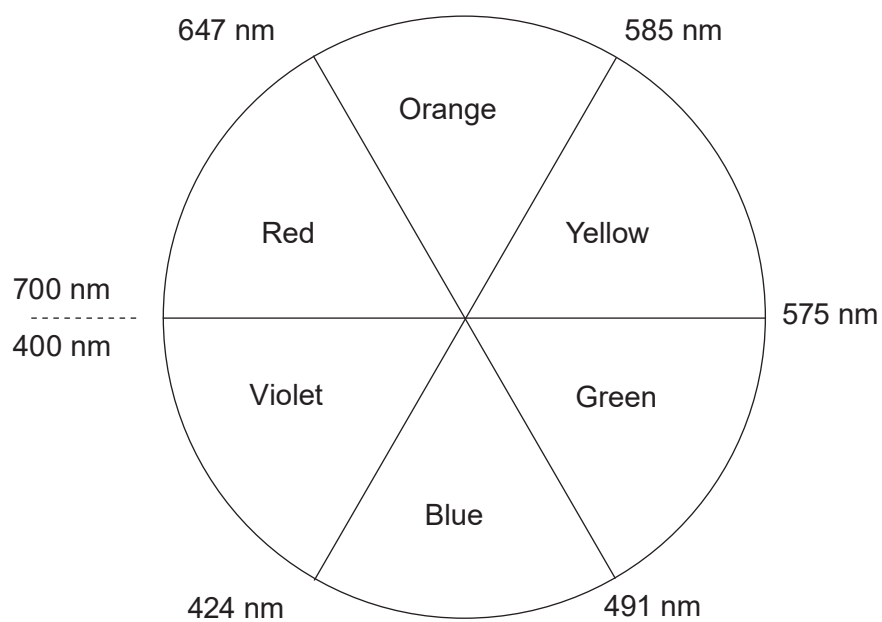
The values of the molar enthalpy of combustion ( $\Delta H_c^\ominus$ ) in the following table refer to a temperature of 298.15 K and a pressure of 100 kPa.

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

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

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## 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

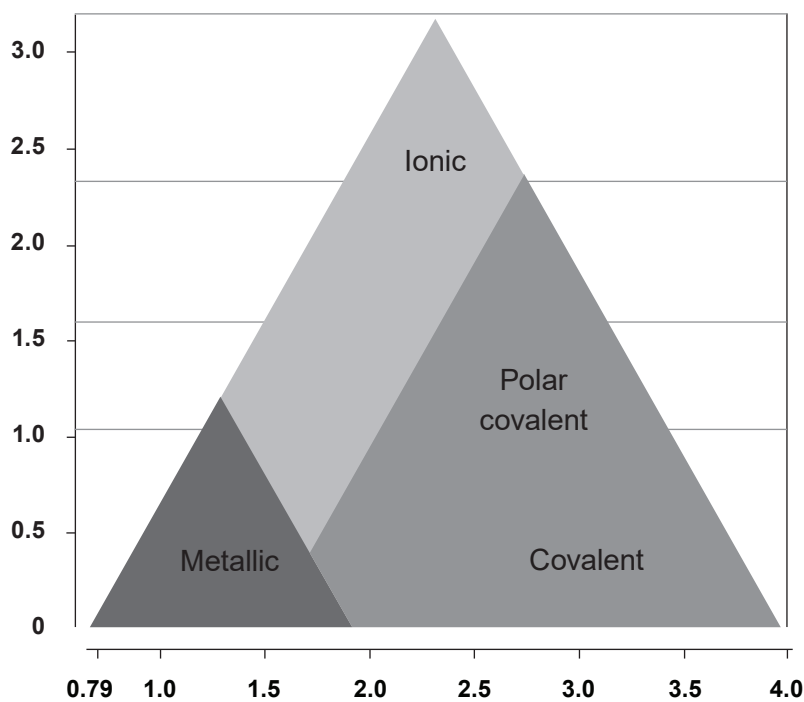
Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$
CaF <sub>2</sub>	2651
BeCl <sub>2</sub>	3033
MgCl <sub>2</sub>	2540
CaCl <sub>2</sub>	2271
SrCl <sub>2</sub>	2170
BaCl <sub>2</sub>	2069
MgO	3791
CaO	3401

Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$
SrO	3223
BaO	3054
CuCl <sub>2</sub>	2824
AgF	974
AgCl	918
AgBr	905
AgI	892

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

Electronegativity difference:

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



%  
covalent

%  
ionic

Average electronegativity:

$$\Sigma\chi = \frac{(\chi_a + \chi_b)}{2}$$

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

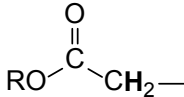
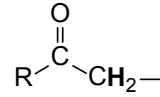
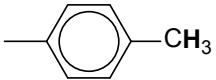
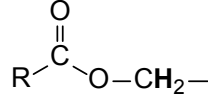
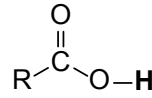
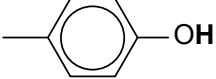

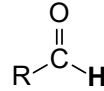
Bond	Types of organic molecules	Wavenumber / $\text{cm}^{-1}$	Intensity
C—I	iodoalkanes	490–620	strong
C—Br	bromoalkanes	500–600	strong
C—Cl	chloroalkanes	600–800	strong
C—F	fluoroalkanes	1000–1400	strong
C—O	alcohols, esters, ethers	1050–1410	strong
C=C	alkenes	1620–1680	medium-weak; multiple bands
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. $^1\text{H}$ NMR data

### Typical proton chemical shift values ( $\delta$ ) 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	$\text{H}_2\text{O}$
28	$\text{CH}_2=\text{CH}_2$ $\text{CO}$
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 $

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## 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.meta-synthesis.com/webbook/30\\_timeline/timeline.html](http://www.meta-synthesis.com/webbook/30_timeline/timeline.html)

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## 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  $191 \times 10^{-12}$  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.