THE UNIVERSITY of York

CHEMISTRY DATA BOOK

October 2011

INTRODUCTION

This Data Book contains a selection of information and data which is relevant to the Chemistry Courses at York.

As far as thermal data is concerned there are often variations in the values cited in the literature. In these instances, one particular set of values has been chosen for display in the tables and, under normal circumstances, no special problems should arise on account of this choice. For precise work, however, it is advisable to consult the extensive tabulations of source material that are available in the Morrell and Whinfield Libraries. The most valuable of these is:

CRC Handbook of Physics and Chemistry

Ed. R C West

A useful compilation and summary of SI conventions is found in Quantities, Units and Symbols in Physical Chemistry, Mills *et. al*., Blackwell (1989).

D K Smith
October, 2011

C O N T E N T S

GREEK ALPHABET

Alpha	A	α	Nu	N	ν
Beta	B	β	Xi	Ξ	ξ
Gamma	Γ	γ	Omicron	O	ο
Delta	Δ	δ	Pi	Π	π
Epsilon	E	ε	Rho	P	ρ
Zeta	Z	ζ	Sigma	Σ	σ
Eta	H	η	Tau	T	τ
Theta	Θ	θ	Upsilon	Y	υ
Iota	I	ι	Phi	Φ	φ
Kappa	K	κ	Chi	X	χ
Lambda	Λ	λ	Psi	Ψ	ψ
Mu	M	μ	Omega	Ω	ω

ATOMIC FIRST IONIZATION ENERGIES (eV)

								H 13.6 He 24.6									
			Li 5.4	Be 9.3	B 8.3	C 11.3	N 14.5	O 13.6	F 17.4	Ne 21.6							
			Na 5.1	Mg 7.6	Al 6.0	S i 8.2	P 10.5	S 10.4	Cl 13.0	Ar 15.8							
			K 4.3	Ca 6.1	Ga 6.0	Ge 8.1	As 9.8	Se 9.8	Br 11.8	Kr 14.0							
			Rb 4.2	Sr 5.7	In 5.8	Sn 7.3	Sb 8.6	Te 9.0	I 10.5	Xe 12.1							
			Cs 3.9	Ba 5.2	Tl 6.1	Pb 7.4	Bi 7.3	Po 8.4	At 10.8	Rn 10.7							
		Sc 6.5	Ti 6.8	V 6.7	Cr 6.8	Mn 7.4	Fe 7.9	Co 7.9	Ni 7.6	Cu 7.7	Zn 9.4						
		Y 6.4	Zr 6.8	Nb 6.9	Mo 7.1	Tc 7.3	Ru 7.4	Rh 7.5	Pd 8.3	Ag 7.6	Cd 9.0						
		La 5.6	Hf 6.6	Ta 7.9	W 8.0	Re 7.9	Os 8.7	Ir 9.1	Pt 9.0	Au 9.2	Hg 10.4						
Ce 5.5	Pr 5.5	Nd 5.5	Pm 5.6	Sm 5.6	Eu 5.7	Gd 6.1	Tb 5.9	Dy 5.9	Ho 6.0	Er 6.1	Tm 6.2	Yb 6.3	Lu 5.4				
Th 6.3	Pa 5.9	U 6.2	Np 6.3	Pu 6.0	Am 6.0	Cm 6.0	Bk 6.2	Cf 6.3	Es 6.4	Fm 6.5	Mv 6.6	No 6.7	Lw 4.9				

ELECTRON-GAIN ENERGIES ΔU_o / kJ mol^{-1}

PERIODIC TABLE ARRANGEMENT						
Li –59.8		B –17.3	C –122.3	N 20.1	O –141.1	F –328.0
Na –52.2		Al –44	Si –133.6	P –72	S –200.4	Cl –348.8
K –45.4	Cu –118		Ge –115	As –77	Se –195.0	Br –324.6
Rb –46.9	Ag –125.7		Sn –120	Sb –100	Te –190.2	I –295.4
Cs –45.5	Au –222.8					

IONIC RADII (in pm - after Shannon and Prewitt)

The values given are applicable to oxides and fluorides (c.n. 6, based on the value 140 pm for 6-coordinated O^{2-}). Radii for other c.n's are given in the Notes below, and the values for species enclosed in the "box" gives an appropriate idea of the sizes of these ions.

Oxidation State	(A) Non-transition Metals								
–3		N 155	P 185	As 220					
–2		O(c) 140	S 185	Se 195	Te 220				
–1		F(d) 133	Cl 180	Br 195	I 220	OH^- 155	SH^- 200		
+1	Li(a) 74	Na 102	K 138	Rb 149	Cs 170	Tl 150	NH_4^+ 150		
+2	Be(b) 35	Mg 72	Ca 100	Sr 116	Ba(e) 136	Zn 75	Cd 105	Pb 118	
+3		Al 53	Sc 89	Y 109	La 115				
+4			Ti 61	Zr 80					

Oxidation State		(B) Transition Metals							
		Ti	V	Cr	Mn	Fe	Co	Ni	Cu
+2	Low spin			73	67	61	65		
	High spin	86	79	82	83	78	75	69	73
+3	Low spin				58	55	55	56	
	High spin	67	64	62	65	65	61	60	-

Notes: (a) c.n. 4, 59 pm
(b) c.n. 4, 27 pm
(c) c.n. 2, 135 pm; c.n. 8, 142 pm
(d) M-F is at least 10 pm greater than M-O in ScOF and YOF (See Wells, p. 404, 4th edn).
(e) c.n. 8, 142 pm; c.n. 12, 160 pm

SINGLE BOND COVALENT RADII (in pm)

H 30	**C** 77	**N** 75	**O** 73	**F** 71
	Si 118	**P** 110	**S** 103	**Cl** 99
	Ge 122	**As** 121	**Se** 117	**Br** 114
	Sn 140	**Sb** 143	**Te** 135	**I** 133

SLATER ATOMIC RADII AND ALLRED-ROCHOW ELECTRONEGATIVITIES

Data are given in the form: Atom Radius/pm
Electronegativity

			H 53 2.20						
Li 145 0.97	Be 105 1.47		B 85 2.01	C 70 2.50	N 65 3.07	O 60 3.50	F 50 4.10		
Na 180 1.01	Mg 150 1.23		Al 125 1.47	Si 110 1.74	P 100 2.0	S 100 2.44	Cl 100 2.83		
K 220 0.91	Ca 180 1.04		Ga 130 1.82	Ge 125 2.02	As 115 2.20	Se 115 2.48	Br 115 2.74		
Rb 235 0.90	Sr 200 0.99		In 155 1.49	Sn 145 1.72	Sb 145 1.82	Te 140 2.01	I 140 2.21		
Cs 260 0.86	Ba 215 0.97		Tl 190 1.44	Pb 180 1.55	Bi 160 1.67	Po 190 1.76	At - 1.90		
Fr - 0.86	Ra 215 0.97	Ac 195 1.00							
. . . . .									
Sc 160 1.20	Ti 140 1.32	V 135 1.45	Cr 140 1.56	Mn 140 1.60	Fe 140 1.64	Co 135 1.70	Ni 135 1.75	Cu 135 1.75	Zn 135 1.66
Y 180 1.11	Zr 155 1.22	Nb 145 1.23	Mo 145 1.30	Tc 135 1.36	Ru 130 1.42	Rh 135 1.43	Pd 140 1.35	Ag 160 1.42	Cd 155 1.46

La	195	Hf	155	Ta	145	W	135	Re	135	Os	130	Ir	135	Pt	135	Au	135	Hg	150
	1.08		1.23		1.33		1.40		1.46		1.52		1.55		1.44		1.41		1.44

. . . . . .

Ce	185	Pr	185	Nd	185	Pm	183	Sm	185	Eu	185	Gd	180			
	1.08		1.07		1.07		1.07		1.07		1.01		1.11			

Tb	175	Dy	175	Ho	175	Er	175	Tm	175	Yb	175	Lu	175			
	1.10		1.10		1.10		1.11		1.11		1.06		1.14			

. . . . . .

Th	180	Pa	180	U	175	Np	175	Pu	175	Am	175					
	1.11		1.14		1.22		1.22		1.22		1.2					

Notes:

(1) The Electronegativities are taken from Table 4.8 of Inorganic Chemistry, by J E Huheey - see also A L Allred and E G Rochow, J. Inorg. Nucl. Chem., 5, 264 (1958) and E J Little and M M Jones, J. Chem. Educ., 27, (1960) for original calculations.

(2) The Atomic Radii are taken from Table 3-1 in Quantum Theory of Molecules and Solids by J C Slater (vol 2).

TABLE OF STANDARD HALF-CELL REDUCTION POTENTIALS

Half-cell reduction potentials in aqueous acid ($a_H = 1.0$) solutions at 298.15 K (25°C) (after W.M. Latimer).

Oxidised/Reduced Species	$E^{\ominus}$ /V		Oxidised/Reduced Species	$E^{\ominus}$ /V
Ag^+/Ag	+ 0.7991		K^+/K	–2.925
Ag^{2+}/Ag^+	+ 1.98			
$AgCl/Ag,\ Cl^-$	+ 0.222		La^{3+}/La	–2.37
$Al^{3+}\ /\ Al$	–1.66		Li^+/Li	–3.045
Au^+/Au	+1.68			
$Au^{3+}\ /\ Au$	+1.50		Mg^{2+}/Mg	–2.37
			Mn^{2+}/Mn	–1.18
Ba^{2+}/Ba	–2.90		Mn^{3+}/Mn^{2+}	+1.51
Be^{2+}/Be	–1.85		$MnO_4^-\ /\ MnO_4^{2-}$	+0.564
$Br_2(\ell)/2Br^-$	+1.0652		$MnO_4^-\ 8H^+/Mn^{2+},\ 4H_2O$	+1.51
			$MnO_4^{2-}, 4H^+/MnO_2, 2H_2O$	+1.695
Ca^{2+}/Ca	–2.76			
Cd^{2+}/Cd	–0.403		Na^+/Na	–2.711
$Cl_2/2Cl^-$	+1.3595		Ni^{2+}/Ni	–0.250

continued ...

Oxidised/Reduced Species	$E^{\ominus}$ /V		Oxidised/Reduced Species	$E^{\ominus}$ /V
Co^{2+}/Co	–0.277		$O_2, 2H^+/H_2O_2$	+0.682
Co^{3+} / Co^{2+}	+1.82		$O_2, 4H^+/2H_2O$	+1.229
Cr^{3+}/Cr	–0.74		$O_3, 2H^+/O_2, H_2O$	+2.07
Cr^{3+}/Cr^{2+}	–0.41		$OH, H^+/H_2O$	+2.8
$Cr_2O_7^{2-},14H^+/2Cr^{3+},7H_2O$	+1.33			
Cs^+/Cs	–2.923		Pb^{2+}/Pb	–0.126
Cu^+/Cu	+0.521		$PbO_2, 4H^+/Pb^{2+}, 2H_2O$	+1.455
Cu^{2+}/Cu	+0.337			
Cu^{2+}/Cu^+	+0.153		Ra^{2+}/Ra	–2.92
			Rb^+/Rb	–2.925
$F_2/2F^-$	+2.87			
$F_2, 2H^+/2HF$ (aq)	+3.06		$S_2O_8^{2-}/S_2O_4^{2-}$	+2.01
Fe^{2+}/Fe	–0.409		Sc^{3+}/Sc	–2.08
Fe^{3+}/Fe^{2+}	+0.771		Sn^{2+}/Sn	–0.136
			Sn^{4+}/Sn^{2+}	+0.15
Ga^{3+}/Ga	–0.53		Sr^{2+}/Sr	–2.89

continued ...

TABLE OF STANDARD HALF-CELL REDUCTION POTENTIALS (continued)

Oxidised/Reduced Species	$E^{\ominus}$ /V		Oxidised/Reduced Species	$E^{\ominus}$ /V
$2H^+/H_2$	0.00		Ti^{2+}/Ti	–1.63
$H^+/H(g)$	–2.10		Ti^{3+}/Ti^{2+}	c –0.37
$\frac{1}{2}H_2/H^-$	–2.25		$(TiIV)^{2+}, 2H^+/Ti^{3+}, H_2O$	+0.1
			$TiO_2 + 4H^+ \rightarrow Ti + 2H_2O$	0.86
H_3BO_3, $3H^+/B\ 3H_2O$	–0.87		Tl^+/Tl	–0.3363
$H_2O_2, H^+/OH^\bullet, H_2O$	+0.72		Tl^{3+}/Tl^+	+1.25
H_2O_2, $2H^+/2H_2O$	+1.77			
$Hg_2^{2+}/2Hg$	+0.789		V^{2+}/V	c –1.18
$2Hg^{2+}/Hg_2^{2+}$	+0.905		V^{3+}/V^{2+}	–0.255
			VO^{2+}, $2H^+/V^{3+}, H_2O$	+0.337
$I_2/2I^-$	+0.5355			
$I^{3-}/3I^-$	+0.536		U^{3+}/U	–1.8
In^{3+}/In	–0.342			
			Zn^{2+}/Zn	–0.763

ENTHALPIES OF FORMATION OF GASEOUS MONATOMIC CATIONS, $\Delta H_f^{\ominus}/(\text{kJ mol}^{-1})$

		H^+ 1537												
Li^+ 687	Be^{2+} 2994													
Na^+ 611	Mg^{2+} 2349	Al^{3+} 5484												
K^+ 514	Ca^{2+} 1926	Sc^{3+} 4651	Ti^{2+} 2451	V^{2+} 2590	Cr^{2+} 2654	Mn^{2+} 2520	Fe^{2+} 2751	Co^{2+} 2842	Ni^{2+} 2932	Cu^+ 1090	Zn^{2+} 2783	Ga^+ 871		
			Ti^{3+} 5110	V^{3+} 5425	Cr^{3+} 5647	Mn^{3+} 5775	Fe^{3+} 5715	Co^{3+} 6080	Ni^{3+} 6332	Cu^{2+} 3054		Ga^{3+} 5824		
Rb^+ 495	Sr^{2+} 1790	Y^{3+} 4218								Ag^+ 1019	Cd^{2+} 2623	In^+ 808	Sn^{2+} 2435	Sb^{3+} 5149
										Ag^{2+} 3100		In^{3+} 5348	Sn^{4+} 9321	
Cs^+ 461	Ba^{2+} 1661	La^{3+} 3896								Au^+ 1262	Hg^{2+} 2890	Tl^+ 778	Pb^{2+} 2373	Bi^{3+} 5005
												Tl^{3+} 5640	Pb^{4+} 9550	
Fr^+ 463	Ra^{2+} 1660													

STANDARD ENTHALPIES OF FUSION AND VAPORIZATION AT THE TRANSITION TEMPERATURE $\Delta_{trs}H^{\ominus}$ / (kJ mol^{-1})

AT	T_m/K	Fusion	T_b/K	Vaporization
Elements				
Ag	1234	11.30	2436	250.6
Ar	83.81	1.118	87.29	6.506
Br_2	265.9	10.57	332.4	29.45
Cl_2	172.1	6.41	239.1	20.41
F_2	53.6	0.26	85.0	3.16
H_2	13.96	0.117	20.38	0.916
He	3.5	0.021	4.22	0.084
Hg	234.3	2.292	629.7	59.30
I_2	386.8	15.52	458.4	41.80
N_2	63.15	0.719	77.35	5.586
Na	371.0	2.601	1156	98.01
O_2	54.36	0.444	90.18	6.820
Xe	161	2.30	165	12.6
K	336.4	2.35	1031	80.23
Inorganic compounds				
CCl_4	250.3	2.47	349.9	30.00
CO_2	217.0	8.33	194.6	25.23 s
CS_2	151.2	4.39	319.4	26.74
H_2O	273.15	6.008	373.15	40.636
				44.016 at 298K
H_2S	187.6	2.377	212.8	18.67
H_2SO_4	283.5	2.56		
NH_3	195.4	5.652	239.7	23.35
Organic compounds				
CH_4	90.68	0.941	111.7	8.18
CCl_4	250.3	2.5	350	30.0
C_2H_4	89.85	2.86	184.6	14.7
C_6H_6	278.61	10.59	353.2	30.8
C_6H_{14}	178	13.08	342.1	28.85
$C_{10}H_8$	354	18.80	490.9	51.51
CH_3OH	175.2	3.16	337.2	35.27
				37.99 at 298K
C_2H_5OH	158.7	4.60	352	43.5

STANDARD ENTHALPIES OF HYDRATION AT INFINITE DILUTION $\Delta_{hyd}H^{\ominus}/(kJ\ mol^{-1})$

	Li^+	Na^+	K^+	Rb^+	Cs^+
F^-	-1026	-911	-828	-806	-782
Cl^-	-884	-783	-685	-664	-640
Br^-	-856	-742	-658	-637	-613
I^-	-815	-701	-617	-596	-572

Entries refer to $X^+(g) + Y^-(g) \rightarrow X^+(aq) + Y^-(aq)$.
Data: Principally J.O'M. Bockris and A K N Reddy, *Modern Electrochemistry*, Vol 1 Plenum Press, New York (1970)

STANDARD ION HYDRATION ENTHALPIES
$\Delta_{hyd}H^{\ominus}/(kJ\ mol^{-1})$ at 298 K

Cations

H^+	-1090	Ag^+	-464	Mg^{2+}	-1920
Li^+	-520	NH_4^+	-301	Ca^{2+}	-1650
Na^+	-405			Sr^{2+}	-1480
K^+	-321			Ba^{2+}	-1360
Rb^+	-300			Fe^{2+}	-1950
Cs^+	-277			Cu^{2+}	-2100
				Zn^{2+}	-2050
				Al^{3+}	-4690
				Fe^{3+}	-4430

Anions

OH^-	-460						
F^-	-506	Cl^-	-364	Br^-	-337	I^-	-296

Entries refer to $X^{++}(g) \rightarrow X^{++}(aq)$ based on $H^+(g) \rightarrow H^+(aq)$
Data: Principally J.O'M. Bockris and A K N Reddy, *Modern Electrochemistry*, Vol 1 Plenum Press, New York (1970)

THERMODYNAMIC DATA FOR ELEMENTS AND INORGANIC COMPOUNDS (all values are for 298K).

	$M/(g\ mol^{-1})$	$\Delta_f H^{\ominus}/(kJ mol^{-1})$	$\Delta_f G^{\ominus}/(JK\ mol^{-1})^{\S}$	$S^{\ominus}_{m\,f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p,m}/(JK^{-1}mol^{-1})$
Argon					
Ar(g)	39.95	0	0	+154.84	+20.786
Bromine					
Br_2(l)	159.82	0	0	+152.23	+75.689
Br_2 (g)	159.82	+30.907	+3.110	+245.46	+36.02
Br(g)	79.91	+111.88	+82.396	+173.02	+20.786
Br^-(g)	79.91	-219.07			
Br^-(aq)	79.91	-121.55	-103.96	+82.4	-141.8
HBr(g)	90.92	-36.40	-53.45	+198.70	+29.142
Carbon (for organic compounds, see Organic Table)					
C(s) (graphite)	12.011	0	0	+5.740	+8.527
C(s) (diamond)	12.011	+1.895	+2.900	+2.377	+6.113
C(g)	12.011	+716.68	+671.26	+158.10	+20.838
CO(g)	28.011	-110.53	-137.17	+197.67	+29.14
CO_2(g)	44.010	-393.51	-394.36	+213.74	+37.11
CO_2(aq)	44.010	-413.80	-385.98	+117.6	
HCN(g)	27.03	+135.1	+124.7	+201.78	+35.86
HCN(l)	27.03	+108.87	+124.97	+112.84	+70..63
CN^-(aq)	26.02	+150.6	+172.4	+94.1	

Inorganic continued ...

	$M/(g\,mol^{-1})$	$\Delta_f H^{\ominus}/(kJ\,mol^{-1})$	$\Delta_f G^{\ominus}/(JK\,mol^{-1})^{\S}$	$S^{\ominus}_{m\,f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p,m}/(JK^{-1}mol^{-1})$
Chlorine					
$Cl_2(g)$	70.91	0	0	+223.07	+33.91
Cl(g)	35.45	+121.68	+105.68	+165.20	+21.840
$Cl^-(g)$	35.45	-233.13			
$Cl^-(aq)$	35.45	-167.16	-131.23	+56.5	-136.4
HCl(g)	36.46	-92.31	-95.30	+186.91	+29.12
HCl(aq)	36.46	-167.16	-131.23	+56.5	-136.4
Copper					
Cu(s)	63.54	0	0	+33.150	+24.44
Cu(g)	63.54	+338.32	+298.58	+166.38	+20.79
$Cu^+(aq)$	63.54	+71.67	+49.98	+40.6	
$Cu^{2+}(aq)$	63.54	+64.77	+65.49	-99.6	
$Cu_2O(s)$	143.08	-168.6	-146.0	+93.14	+63.64
Cu(O(s)	79.54	-157.3	-129.7	+42.63	+42.30
Deuterium					
$D_2(g)$	4.028	0	0	+144.96	+29.20
HD(g)	3.022	+0.318	-1.464	+143.80	+29.196
$D_2O(g)$	20.028	-249.20	-234.54	+198.34	+34.27
$D_2O(l)$	20.028	-294.60	-243.44	+75.94	+84.35
HDO(g)	19.022	-245.30	-233.11	+199.51	+33.81
HDO(l)	19.022	-289.89	-241.86	+79.29	

Inorganic continued ...

	$M/(g\,mol^{-1})$	$\Delta_f H^{\ominus}/(kJ mol^{-1})$	$\Delta_f G^{\ominus}/(JK\,mol^{-1})^{\S}$	$S^{\ominus}_{m\,f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p,m}/(JK^{-1}mol^{-1})$
Fluorine					
$F_2(g)$	38.00	0	0	+202.78	+31.30
F(g)	19.00	+78.99	+61.91	+158.75	+22.74
HF(aq)	19.00	-332.63	-278.79	-13.8	-106.7
HF(g)	20.01	-271.1	-273.2	+173.78	29.13
Helium					
He(g)	4.003	0	0	+126.15	+20.786
Hydrogen (see also deuterium)					
$H_2(g)$	2.016	0	0	+130.684	+28.824
H(g)	1.008	+217.97	+203.25	+114.71	+20.784
$H^+(aq)$	1.008	0	0	0	0
$H^+(g)$	1.008	+1536.20			
$H_2O(s)$	18.015			+37.99	
$H_2O(l)$	18.015	-285.83	-237.13	+69.91	+75.291
$H_2O(g)$	18.015	-241.82	-228.57	+188.83	+33.58
$H_2O_2(l)$	34.015	-187.78	-120.35	+109.6	+89.1
Iodine					
$I_2(s)$	253.81	0	0	+116.135	+54.44
$I_2(g)$	253.81	+62.44	+19.33	+260.69	+36.90
I(g)	126.90	+106.84	+70.25	+180 .79	+20.786
$I^-(aq)$	126.90	-55.19	-51.57	+111.3	-142.3
HI(g)	127.91	+26.48	+2.13	+206.59	+29.158

Inorganic continued ...

	$M/(g\ mol^{-1})$	$\Delta_f H^{\ominus}/(kJ mol^{-1})$	$\Delta_f G^{\ominus}/(JK\ mol^{-1})^{\S}$	$S^{\ominus}_{m\,f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p,m}/(JK^{-1}mol^{-1})$
Iron					
Fe(s)	55.85	0	0	+27.28	+25.10
Fe(g)	55.85	+416.3	+370.7	+180.49	+25.68
Fe^{2+}(aq)	55.85	-89.1	-78.90	-137.7	
Fe^{3+}(aq)	55.85	-48.5	-4.7	-315.9	
Fe_3O_4(s) (magnetite)	231.54	-1118.4	-1015.4	+146.4	+143.43
Fe_2O_3(s) (haematite)	159.69	-824.2	-742.2	+87.40	+103.85
Krypton					
Kr(g)	83.80	0	0	+164.08	+20.786
Lithium					
Li(s)	6.94	0	0	+29.12	+24.77
Li(g)	6.94	+159.37	+126.66	+138.77	+20.79
Li^{+}(aq)	6.94	-278.49	-293.31	+13.4	+68.6
Neon					
Ne(g)	20.18	0	0	+146.33	+20.786

Inorganic continued ...

	$M/(g\,mol^{-1})$	$\Delta_f H^{\ominus}/(kJ mol^{-1})$	$\Delta_f G^{\ominus}/(JK\,mol^{-1})^{\S}$	$S^{\ominus}_{m\,f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p,m}/(JK^{-1}mol^{-1})$
Nitrogen					
$N_2(g)$	28.013	0	0	+191.61	+29.125
$N(g)$	14.007	+472.70	+455.56	+153.30	+20.786
$NO(g)$	30.01	+90.25	+86.55	+210.76	+29.844
$N_2O(g)$	44.01	+82.05	+104.20	+219.85	+38.45
$NO_2(g)$	46..01	+33.18	+51.31	+240.06	+37.20
$HNO_3(l)$	63.01	-174.10	-80.71	+155.60	+109.87
$HNO_3(aq)$	63.01	-205.36	-111.25	+146.4	-86.6
$NO_3^-(aq)$	62.01	-205.0	-108.74	+146.4	-86.6
$NH_3(g)$	17.03	-46.11	-16.45	+192.45	+35.06
$NH_3(aq)$	17.03	-80.29	-26.50	+111.3	
$NH_4^4(aq)$	18.04	-132.51	-79.31	+113.4	+79.9
$NH_4NO_3(s)$	80.04	-365.56	-183.87	+151.08	+84.1
$NH_4Cl(s)$	53.49	-314.43	-202.87	+94.6	
Oxygen					
$O_2(g)$	31.999	0	0	+205.138	+29.355
$O(g)$	15.999	+242.17	+231.73	+161.06	+21.912
$O_3(g)$	47.998	+142.7	+163.2	+238.93	+39.20
$OH^-(aq)$	17.007	-229.99	-157.24	-10.75	-148.5

Inorganic continued ...

	$M/(g\,mol^{-1})$	$\Delta_f H^{\ominus}/(kJ\,mol^{-1})$	$\Delta_f G^{\ominus}/(JK\,mol^{-1})^{\S}$	$S^{\ominus}_{m\,f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p,m}/(JK^{-1}mol^{-1})$
Phosphorus					
P(s, wh)	30.97	0	0	+41.09	+23.840
P(g)	30.97	+314.64	+278.25	+163.19	+23.840
P_2(g)	61.95	+144.3	+103.7	+218.13	+32.05
P_4(g)	123.90	+58.91	+24.44	+279.98	+67.15
PH_3(g)	34.00	+5.4	+13.4	+210.23	+37.11
PCl_3(g)	137.33	-287.0	-267.8	+311.78	+71.84
PCl_3(l)	137.33	-319.7	-272.3	+217.1	
Potassium					
K(s)	39.10	0	0	+64.18	+29.58
K(g)	39.10	+89.24	+60.59	+160.336	+20.786
K^+(g)	39.10	+514.26			
K^+(aq)	39.10	-252.38	-283.27	+102.5	+21.8
KOH(s)	56.11	-424.76	-379.08	+78.9	+64.9
KF(s)	58.10	-576.27	-537.75	+66.57	+49.04
KCl(s)	74.56	-436.75	-409.14	+82.59	+51.30
KBr(s)	119.01	-393.80	-380.66	+95.90	+52.30
Kl(s)	166.01	-327.90	-324.89	+106.32	+52.93

Inorganic continued ...

	$M/(g\ mol^{-1})$	$\Delta_f H^{\ominus}/(kJ mol^{-1})$	$\Delta_f G^{\ominus}/(JK\ mol^{-1})^{\S}$	$S^{\ominus}_{m_f}/(JK^{-1}mol^{-1})^{\S}$	$C^{\ominus}_{p.m}/(JK^{-1}mol^{-1})$
Silicon					
Si(s)	28.09	0	0	+18.83	+20.00
Si(g)	28.09	+455.6	+411.3	+167.97	+22.25
$SiO_2(s,\alpha)$	60.09	-910.94	-856.64	+41.84	+44.43
Sodium					
Na(s)	22.99	0	0	+51.21	+28.24
Na(g)	22.99	+107.32	+76.76	+153.71	+20.79
$Na^+(aq)$	22.99	-240.12	-261.91	+59.0	+46.4
NaOH(s)	40.00	-425.61	-379.49	+64.46	+59.54
NaCl(s)	58.44	-411.15	-384.14	+72.13	+50.50
NaBr(s)	102.90	-361.06	-384..98	+86.82	+51.38
NaI(s)	149.89	-287.78	-286.06	+98.53	+52.09
Sulfur					
$S(s,\alpha)$(rhombic)	32.06	0	0	+31.80	+22.64
$S(s,\beta)$(monoclinic)	32.06	+0.33	+0.1	+32.6	+23.6
$S^{2-}(ag)$	32.06	+33.1	+85.8	-14.6	
$SO_2(g)$	64.06	-296.83	-300.19	+248.22	+39.87
$SO_3(aq)$	80.06	-395.72	-371.06	+256.76	+50.67

HEATS OF COMBUSTION

Compound	Formula	Heat of Combustion at 298 K (25°C)/kJ mol^{-1}			
		$H_2O(l) + CO_2(g)$		$H_2O(g) + CO_2(g)$	
Hydrogen	H_2	286	(143.0)	242	(11.0)
Carbon	C	394	(32.8)	394	(32.8)
Carbon Monoxide	CO	283	(10.1)	283	(10.1)
Methane	CH_4	890	(55.6)	802	(50.1)
Ethane	C_2H_6	1560	(52.0)	1428	(47.6)
Ethene	C_2H_4	1411	(50.4)	1323	(47.3)
Ethyne	C_2H_2	1300	(50.0)	1256	(48.3)
Propane	C_3H_8	2221	(50.5)	2044	(46.5)
Propene	C_3H_6	2059	(49.0)	1927	(45.9)
Butane	C_4H_{10}	2879	(49.6)	2659	(45.8)
Hexane	C_6H_{14}	4164	(48.4)	3856	(44.8)
Cyclohexane	C_6H_{12}	3921	(46.7)	3657	(43.5)
Benzene	C_6H_{16}	3268	(41.9)	3136	(40.2)
Octane	C_8H_{18}	5472	(48.0)	5076	(44.5)
2-Methyl-3-ethylpentane	C_8H_{18}	5472	(48.0)	5076	(44.5)
1,4-Dimethylbenzene	C_8H_{10}	4554	(43.0)	4334	(40.9)
Dodecane	$C_{12}H_{26}$	8088	(47.6)	7516	(44.2)
Eicosane	$C_{20}H_{42}$	13320	(47.2)	12395	(44.0)
Ethanol	C_2H_6O	1367	(29.7)	–	–
Ethanal	C_2H_4O	1167	(26.5)	–	–
Ethanoic Acid	$C_2H_4O_2$	875	(14.6)	–	–
Propanone	C_3H_6O	1791	(30.9)	–	–
Phenol	C_6H_6O	3054	(32.5)	–	–

The left- and right- columns of values represent gross and nett calorific values respectively; the values in brackets are the corresponding heats of combustion measured in MJ kg^{-1}.

THERMODYNAMIC DATA FOR ORGANIC COMPOUNDS (ALL VALUES ARE FOR 298K).

	M/(g mol^{-1})	$\Delta_t H^{\ominus}$/(kJmol^{-1})	$\Delta_t G^{\ominus}$/(JK mol^{-1})§	$S^{\ominus}_{m\,t}$/(JK^{-1}mol^{-1})§	$C^{\ominus}_{p.m}$/(JK^{-1}mol^{-1})
C(s) graphite	12.011	0	0	5.740	8.527
C(s) diamond	12.011	+ 1.895	+2.900	2.377	6.113
CO_2(g)	44.041	-393.51	-394.36	213.74	37.11
Hydrocarbons					
CH_4(g) methane	16.04	-74.81	-50.72	186.26	35.31
CH_3(g) methyl	15.04	+145.69	+147.92	194.2	38.70
C_2H_2(g) ethyne	26.04	+226.71	+209.20	200.94	43.93
C_2H_4(g) ethene	28.05	+52.26	+68.15	219.56	43.56
C_2H_6(g) ethane	30.07	-84.68	-32.82	229.60	52.63
C_3H_6(g propene	42.08	+20.42	+62.78	267.05	63.89
C_3H_6 (g) cyclopropane	42.08	+53.30	+104.45	237.55	55.94
C_3H_8 (g) propane	44.10	-103.85	-23.49	269.91	73.5
C_4H_8 (g) 1-butene	56.11	-0.13	+71.39	305.71	85.65
C_4H_8 (g) *Z*-2-butene	56.11	-6.99	+65.95	300.94	78.91
C_4H_8 (g) *E*-2-butene	56.11	-11.17	+63.06	296.59	87.82
C_4H_{10}(g) butane	58.13	-126.15	-17.03	310.23	97.45
C_5H_{12} (g) pentane	72.15	-146.44	-8.20	348.40	120.2
C_5H_{12} (l)	72.15	-173.1			
C_6H_6(l) benzene	78.12	+49.0	+124.3	173.3	136.1
C_6H_6 (g)	78.12	+82.93	+129.72	269.31	81.67
C_6H_{12} (l) cyclohexane	84.16	-156	+26.8	204.4	156.5
$C_6H_5CH_3$ (g) toluene	92.14	-198.7		204.3	
$C_6H_5CH_3$(l)	92.14	+50.5	+122.0	320.7	103.6

	M/(g mol^{-1})	$\Delta_t H^{\ominus}$/(kJmol^{-1})	$\Delta_t G^{\ominus}$/(JK mol^{-1})[§]	$S^{\ominus}_{m\,t}$/(JK^{-1}mol^{-1})[§]	$C^{\ominus}_{p.m}$/(JK^{-1}mol^{-1})
Alcohols and Phenols					
CH_3OH(l) methanol	32.04	-238.66	-166.27	126.8	81.6
C_5H_5OH(l) ethanol	46.07	-277.69	-174.78	160.7	111.46
C_6H_5OH(s) phenol	94.12	-165.0	-50.9	146.0	
Carboxylic acids					
HCOOH(l) formic	46.03	-424.72	-361.35	128.95	99.04
CH_3COOH(l)acetic	60.05	-484.5	-389.9	159.8	124.3
CH_3COOH(aq)	60.05	-485.76	-396.46	178.7	
$(COOH)_2$(s) oxalic	90.04	-872.2			117
C_6H_5COOH(s) benzoic	122.13	-385.1	-245.3	167.6	146.8
Nitrogen Compounds					
$CO(NH_2)_2$(s) urea	60.06	-333.51	-197.33	104.60	93.14
CH_2NH_2(g) methylamine	31.06	-22.97	+32.16	243.41	53.1

PROPERTIES OF SELECTED ORGANIC COMPOUNDS

	Melting Point T_m/K	Boiling Point T_b/K	Density* ρ/kg m^{-3} (at 293 K)	Enthalpy of formation *§ ΔH_f° / kJ mol^{-1}	State
Benzene	279	353	879	+49	l
Benzoic Acid	396	522	1266	–392	s
Bromomethane	180	277	1676	–36	g
Butane	135	273	579	–146	l
Butanoic acid	269	437	958	–539	l
Chloromethane	175	249	916	–82	g
Cyclohexane	280	354	779	–154	l
Cyclohexanol	297	434	962	–351	l
Dichloromethane	178	313	1327	–121	l
Dodecane	263	489	749	–291	l
Ethanal	152	294	783	–192	g
Ethane	90	185	545++	–85	g
Ethanoic acid	290	391	1049	–485	l
Ethanol	156	352	789	–278	l
Ethene	104	169	567§§	+52	g
Ethoxyethane	157	308	714	–280	l
Ethyne	192	189		+227	g
Heptane	183	372	638	–224	l
Hexane	178	342	660	–199	l
Iodomethane	207	316	2279	–8	l

	Melting Point T_m/K	Boiling Point T_b/K	Density* ρ/kg m^{-3} (at 293 K)	Enthalpy of formation *§ ΔH_f° / kJ mol^{-1}	State
Methane	91	109	423+	–75	g
Methanol	179	338	791	–239	l
Methoxymethane	135	250		–184	g
Methylbenzene	178	384	867	+12	l
2-methylpropane	114	261	557	–135	g
Octane	216	399	702	–250	l
Pentane	143	309	626	–173	l
Propane	83	231	493	–105	g
Propane-1,2,3-triol	293	decomp.**	1261	–104	l
Propanoic acid	252	414	993	–509	l
Propanol	147	371	803	–302	l
Propanone	178	329	790	–217	l
Propene	88	226	505	+20	g
Tetrachloromethane	250	350	1594	–136	l
Trichloromethane	210	335	1483	–134	l
1,2-Dimethylbenzene	248	417	880	+79	l
1,3-Dimethylbenzene	225	412	864	+72	l
1,4-Dimethylbenzene	286	411	861	+75	l

* At 298 K; § A negative sign means evolution of heat; ** At 453 K

\+ At 111.5 K ++ At 184 K §§ At 104 K

TEMPERATURE, PRESSURE AND VOLUME RELATIONSHIP OF SATURATED STEAM

Temperature T/K	Temperature (^oC)	Pressure P/bar** abs	Specific volume $V/m^3\ kg^{-1}$
273	(0)	0.00611	206
283	(10)	0.0123	106
293	(20)	0.0234	57.8
298	(25)	0.0317	43.4
303	(30)	0.0424	32.9
323	(50)	0.123	12.0
343	(70)	0.312	5.05
363	(90)	0.701	2.36
368	(95)	0.845	1.98
373	(100)	1.01	1.67
383	(110)	1.43	1.21
393	(120)	1.98	0.892
403	(130)	2.70	0.669
413	(140)	3.61	0.509
423	(150)	4.76	0.393
433	(160)	6.18	0.307
443	(170)	7.92	0.243
453	(180)	10.0	0.194
463	(190)	12.6	0.156
473	(200)	15.6	0.127
498	(225)	25.5	0.0783
523	(250)	39.8	0.0500
548	(275)	59.5	0.0327
573	(300)	85.9	0.0216
598	(325)	121	0.0142
623	(350)	165	0.0088
647*	(374)	221	0.00316

* Critical point ** 1 bar = 10^5 N m^{-2}

THERMAL PROPERTIES OF LIQUID WATER
(AT 1 ATMOSPHERE PRESSURE)

Temperature T/K	(^oC)	Density ρ/kg m^{-3}	Specific Heat Capacity C_p/J kg^{-1} K^{-1}	Specific Latent Heat of Vaporisation ℓ/kJ kg^{-1}
273	(0)	999.9	4217	2493
283	(10)	999.7	4192	2469
293	(20)	998.2	4182	2446
303	(30)	995.7	4178	
313	(40)	992.2	4178	2400
323	(50)	988.1	4180	
333	(60)	983.2	4184	2353
343	(70)	977.8	4189	
353	(80)	971.8	4196	2307
363	(90)	965.3	4205	
373	(100)	958.4	4216	2260
398	(125)	938.8*		
423	(150)	916.9*		
448	(175)	892.4*		
473	(200)	864.5*		

* At appropriate pressure - see Table pertaining to steam.

TABLE OF ENERGY EQUIVALENTS

Energy associated with	J	eV	calories	kW h	Hz	cm^{-1}	K	$J\ mol^{-1}$
1 Joule (J)	1	6.242×10^{18}	0.2390	2.778×10^{-7}	1.509×10^{33}	5.034×10^{22}	7.244×10^{22}	6.022×10^{23}
1 eV	1.602×10^{-19}	1	3.829×10^{-20}	4.450×10^{-26}	2.418×10^{14}	8.066×10^{3}	1.160×10^{4}	9.649×10^{4}
1 calorie	4.184	2.612×10^{17}	1	1.162×10^{-6}	6.317×10^{33}	2.107×10^{23}	3.030×10^{23}	2.520×10^{22}
1 kilowatt-hour (kW h)	3.600×10^{6}	2.2247×10^{25}	8.604×10^{5}	1	5.432×10^{39}	1.812×10^{29}	2.608×10^{29}	2.168×10^{28}
1 Hertz (Hz)	6.262×10^{-34}	4.136×10^{-15}	1.583×10^{36}	1.841×10^{-40}	1	3.336×10^{-11}	4.800×10^{-11}	3.990×10^{-10}
1 reciprocal centimetre	1.986×10^{-23}	1.240×10^{-4}	4.747×10^{-24}	5.517×10^{-30}	2.997×10^{10}	1	1.439	1.196×10^{1}
1 Kelvin (K)	1.381×10^{-23}	8.620×10^{-5}	3.301×10^{24}	3.836×10^{-30}	2.084×10^{10}	6.952×10^{1}	1	8.316
1 Therm	1.055×10^{8}							1

APPROXIMATE VALUE OF AN EINSTEIN

λ/nm	200	300	400	500	600	700
$Nh\nu$/kJ mol^{-1}	600	400	300	240	200	170

APPROXIMATE ENERGY CONVERSION FACTORS

To convert from one fuel/unit (down the left hand side) to another, (across the top of the Table) multiply by the factor shown:
e.g. 1 t oil eq ≡ 397 therms ≡ 11.63 MW h ≡ 41.87 GJ

From ↓ / **To →**	**t oil eq**	**therms**	**MW h**	**GJ**
t oil eq	1	397	11.63	41.87
10^3 therms	2.52	1000	29.3	105.5
MW h	0.086	34.1	1	3.60
TJ	23.9	9480	278	1000

1 t oil equivalent is a unit of energy, defined as the gross calorific value of a notional grade of crude petroleum.

Conversions between any of therms, MW h and GJ are precise (independent of assumptions about fossil fuels).

The calorific value of coal varies with its source/quality. The gross calorific value of coal burned in the UK is typically between 25 - 30 GJ t^{-1}.

For electricity generated (MW h) from fossil fuels you need to take into account the calorific value of the fuel and the thermal efficiency of conversion.

For conversions between J and eV, see Table of Energy Equivalents.

For conversions between mass and energy, $E = mc^2$,

1 amu = 931.5 MeV

THE EARTH

Radius (mean)	=	6371 km
(polar)	=	6357 km
(equatorial)	=	6378 km
Surface area	=	5.1×10^{14} m^2
Greatest height (Mt Everest)	=	8848 m
Greatest depth (Mariana Trench)	=	11020 m
Land area	=	150×10^6 km^2
Ocean area	=	360×10^6 km^2
Volume	=	1.08×10^{21} m^3
Mass	=	5.98×10^{24} kg
Density (mean	=	5520 kg m^{-3}
Gravitational acceleration, g		
at surface (mean)	=	9.81 m s^{-2}
(polar)	=	9.85 m s^{-2}
(equatorial)	=	9.75 m s^{-2}

$g/\text{m s}^{-2} = 9.80616 - 0.025928 \cos 2\lambda + 0.000069 \cos^2 2\lambda - 0.000003h$

where λ is the latitude and h the height above sea-level

Moment of inertia about axis of rotation	=	8×10^{37} kg m^2
Velocity (escape, at surface)	=	11 km s^{-1}
(rotational, at equator)	=	0.4 km s^{-1}
Solar flux (mean)	=	1.40 kW m^{-2}

UK LAND STATISTICS

Total area	24.8×10^{10} m^2
Urban	3.5×10^{10} m^2
Water or river	0.3×10^{10} m^2
Woodland	2.0×10^{10} m^2
Rough Grazing	6.7×10^{10} m^2
Arable	4.9×10^{10} m^2
Temporary grass	2.4×10^{10} m^2
Permanent grass	5.0×10^{10} m^2
1 ha = 10^4 m^2 = 2.47 acres	

THE ATMOSPHERE

Composition of dry air (by volume) :
N_2 (78%); O_2 (21%); Ar (0.93%); CO_2 (0.037%);
Ne, He, CH_4, Kr, H_2, N_2O, Xe, Rn (all in very small amounts - total 0.003%)

The moisture content of 100% humidity air:
0.60% at 0^{o}C 1.20% at 10^{o}C 1.68% at 15^{o}C 2.32% at 20^{o}C

THE GEOLOGICAL TIME SCALE

After W B Harland, R L Armstrong, L E Craig, A G Smith and D G Smith (1990). *A Geological Time Scale 1989*, Cambridge University Press

Eon	Era	Period	Sub-Period	Epoch*	Age/ Ma†
Phanerozoic	Cenozoic	Quaternary		Holocene	0.01
				Pleistocene	1.64
		Tertiary	Neogene	Pliocene	5.2
				Miocene	23.5
			Palaeogene	Oligocene	35.5
				Eocene	56.5
				Palaeocene	65.0
	Mesozoic	Cretaceous		Senonian	88.5
				Gallic	131.8
				Neocomian	145.6
		Jurassic		Malm	157.1
				Dogger	178.0
				Lias	208.0
		Triassic			245.0
	Palaeozoic	Permian		Zechstein	256.1
				Rotliegendes	290.0
		Carboniferous			362.5
		Devonian			408.5
		Silurian			439.0
		Ordovician			510.0
		Cambrian			570
Proterozoic					2500
Archaean					3800
Hadean					4560

Notes:

* Epoch names are given only for the Permian, Jurassic, Cretaceous, Tertiary and Quaternary

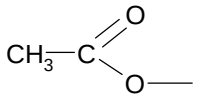
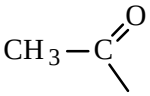
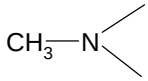
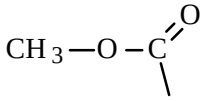
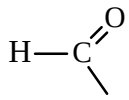
† Ma - Mega annum

1 The Hadean, Archaean and Proterozoic together are commonly called Precambrian.

2 The Cambrian, Ordovician and Silurian are commonly classified as Lower Palaeozoic; and the Devonian, Carboniferous and Permain as Upper Palaeozoic.

3 Probable age of the Earth - 4560 Ma; oldest dated rocks about 3800 Ma.

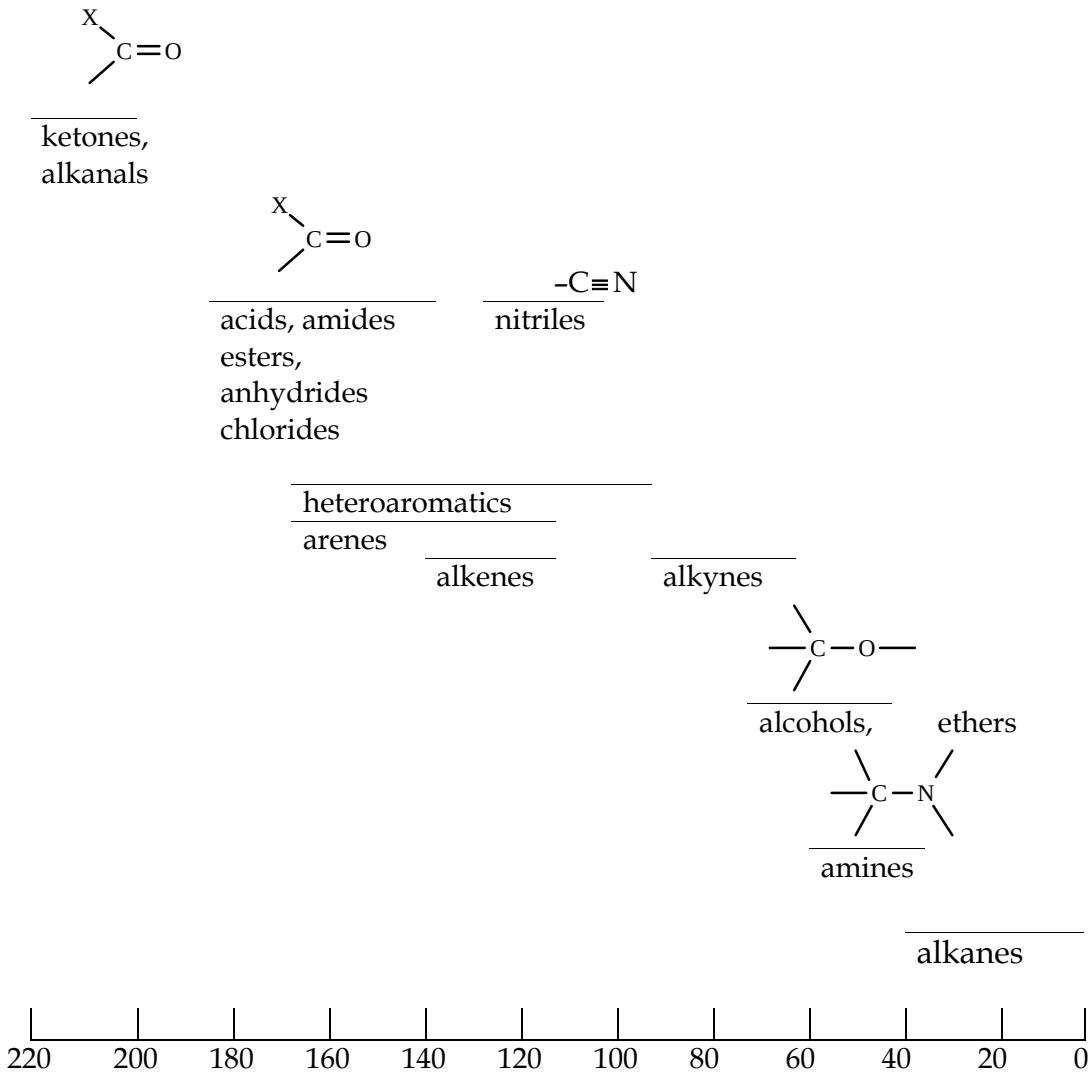
TYPICAL VALUES OF ^1H ATOM CHEMICAL SHIFTS/δ*

Group	Type of Compound	Chemical Shift δ*
CH_3–Si	methylsilane	0.0
CH_3–C	alkane	0.9
C–CH_2–C	alkane	1.3
CH_3–C=C	alkene	1.6
	ester, acid	2.0
	ketone	2.2
CH_3–Ar	alkyl arene	2.3
CH_3–S–	methyl thioether	2.1
HC≡C–	alkyne	2.0‡
	amine	2.3
CH_3–O–	methyl ether	3.3
	methyl ester	3.7
CH_2=C	alkene	4.7‡
	arene	7.3‡
	alkanal	9.7‡
H–M	metal hydride complexes	-2 → –30
CH_3–M	metal alkyl complexes	1 → –2
CH_3 –I	iodoalkane	2.2
CH_3–Br	bromoalkane	2.6
CH_3–Cl	chloroalkane	3.0
CH_3–F	fluoroalkane	4.3

* Typically ± 0.1δ

‡ Substituent effects may cause a significant variation in the value listed.

RANGES OF SOME ^{13}C NMR CHEMICAL SHIFTS



NMR PROPERTIES AND RELATIVE ATOMIC MASSES OF STABLE SINGLE ISOTOPES

Species	% Natural Abundance	Relative Isotopic Mass M/g mol^{-1}	Nuclear Spin, I	Frequency/MHz at 7.046 T
^{1}n	0.000	1.009	1/2	205.607
^{1}H	99.984	1.008	1/2	300.130
^{2}H	0.016	2.014	1	46.073
^{3}H	0.000	3.016	1/2	320.128
^{3}He	1.3×10^{-4}	3.016	1/2	228.633
^{4}He	100.000	4.003	0	
^{6}Li	7.420	6.015	1	44.167
^{7}Li	92.580	7.016	3/2	116.640
^{9}Be	100.000	9.012	3/2	42.174
^{10}B	19.580	10.013	3	32.246
^{11}B	80.420	11.009	3/2	96.258
^{12}C	98.890	12.000	0	
^{13}C	1.108	13.003	1/2	75.468
^{14}N	99.630	14.003	1	21.687
^{15}N	0.370	15.000	1/2	30.424
^{16}O	99.760	15.995	0	
^{17}O	0.037	16.999	5/2	40.686
^{18}O	0.204	17.999	0	
^{19}F	100.000	18.998	1/2	282.404
^{21}Ne	0.257	20.994	3/2	23.692
^{23}Na	100.000	22.990	3/2	79.390
^{25}Mg	10.130	24.986	5/2	18.374
^{27}Al	100.000	26.982	5/2	78.205
^{28}Si	92.230	27.977	0	
^{29}Si	4.670	28.976	1/2	59.627
^{30}Si	3.100	29.974	2	
^{31}P	100.000	30.974	1/2	121.496
^{32}S	95.000	31.972	0	
^{33}S	0.760	32.971	3/2	23.038
^{34}S	4.220	33.968	0	
^{35}Cl	75.530	34.969	3/2	29.407
^{37}Cl	24.470	36.966	3/2	24.479
^{39}K	93.080	38.964	3/2	14.004

Species	% Natural Abundance	Relative Isotopic Mass M/g mol^{-1}	Nuclear Spin, I	Frequency/MHz at 7.046 T
^{41}K	6.880	40.962	3/2	7.686
^{43}Ca	0.145	42.959	7/2	20.196
^{45}Sc	100.000	44.956	7/2	72.908
^{47}Ti	7.280	46.952	5/2	16.924
^{49}Ti	5.510	48.948	7/2	16.920
^{50}V	0.240	49.947	6	29.923
^{51}V	99.760	50.944	7/2	78.943
^{53}Cr	9.550	52.941	3/2	16.963
^{55}Mn	100.000	54.938	5/2	74.267
^{57}Fe	2.190	56.935	1/2	9.718
^{59}Co	100.000	58.933	7/2	71.212
^{61}Ni	1.190	60.931	3/2	26.820
^{63}Cu	69.090	62.930	3/2	79.618
^{65}Cu	30.910	64.928	3/2	85.288
^{67}Zn	4.110	66.927	5/2	18.779
^{69}Ga	60.400	68.926	3/2	72.034
^{71}Ga	39.600	70.925	3/2	91.531
^{73}Ge	7.760	72.923	9/2	10.469
^{75}As	100.000	74.922	3/2	51.391
^{77}Se	7.580	76.920	1/2	57.241
^{79}Br	50.540	78.918	3/2	75.195
^{81}Br	49.460	80.916	3/2	81.056
^{83}Kr	11.550	82.914	9/2	11.542
^{85}Rb	72.150	84.912	5/2	28.965
^{87}Rb	27.850	86.909	3/2	98.206
^{87}Sr	7.020	86.909	9/2	13.008
^{89}Y	100.000	88.906	1/2	14.706
^{91}Zr	11.230	90.905	5/2	27.900
^{93}Nb	100.000	92.906	9/2	73.460
^{95}Mo	15.720	94.906	5/2	19.559
^{97}Mo	9.460	97.906	5/2	19.971
^{99}Tc	100.000	98.906	9/2	67.553
^{99}Ru	12.720	98.906	3/2	10.169
^{101}Ru	17.070	100.906	5/2	14.824
^{103}Rh	100.000	102.904	1/2	9.559
^{105}Pd	22.300	104.904	5/2	13.734

Species	% Natural Abundance	Relative Isotopic Mass M/g mol^{-1}	Nuclear Spin, I	Frequency/MHz at 7.046 T
^{107}Ag	51.580	106.905	1/2	12.149
^{109}Ag	48.180	108.904	1/2	13.968
^{111}Cd	12.750	110.904	1/2	63.631
^{113}Cd	12.260	112.904	1/2	66.563
^{113}In	4.280	112.904	9/2	65.626
^{115}In	95.720	114.904	9/2	65.767
^{117}Sn	7.610	116.903	1/2	106.942
^{119}Sn	8.580	118.903	1/2	111.921
^{121}Sb	57.250	120.903	5/2	71.824
^{123}Sb	42.750	122.904	7/2	38.894
^{123}Te	0.870	122.904	1/2	78.544
^{125}Te	6.990	124.904	1/2	94.691
^{127}I	100.000	126.904	5/2	60.053
^{129}Xe	26.440	128.904	1/2	83.010
^{131}Xe	21.180	130.905	3/2	24.611
^{133}Cs	100.000	132.905	7/2	39.865
^{135}Ba	6.590	134.905	3/2	29.815
^{137}Ba	11.320	136.905	3/2	33.353
^{138}La	0.089	137.905	5	39.599
^{139}La	99.911	138.908	7/2	42.396
^{141}Pr	100.000	140.907	5/2	87.911
^{143}Nd	12.170	142.909	7/2	16.318
^{145}Nd	8.300	144.912	7/2	10.039
^{147}Sm	14.950	146.915	7/2	12.389
^{149}Sm	13.830	148.912	7/2	9.871
^{151}Eu	47.820	150.920	5/2	74.435
^{153}Eu	52.180	152.921	5/2	32.867
^{155}Gd	14.730	154.922	3/2	11.462
^{157}Gd	15.680	156.923	3/2	14.328
^{159}Tb	100.000	158.925	3/2	68.063
^{161}Dy	18.880	160.927	5/2	9.886
^{163}Dy	24.970	162.929	5/2	13.755
^{165}Ho	100.000	164.930	7/2	61.566
^{167}Er	22.940	166.932	7/2	8.674
^{169}Tm	100.000	168.934	1/2	24.824
^{171}Yb	14.310	170.936	1/2	52.862

Species	% Natural Abundance	Relative Isotopic Mass M/g mol^{-1}	Nuclear Spin, I	Frequency/MHz at 7.046 T
^{173}Yb	16.130	172.938	5/2	14.562
^{175}Lu	97.410	174.941	7/2	34.236
^{176}Lu	2.590	175.943	7	23.794
^{177}Hf	18.500	176.943	7/2	9.364
^{179}Hf	13.750	178.946	9/2	5.609
^{181}Ta	99.988	180.948	7/2	35.986
^{183}W	14.400	182.950	1/2	12.503
^{185}Re	37.070	184.953	5/2	67.604
^{187}Re	62.930	186.956	5/2	68.286
^{187}Os	1.640	186.956	1/2	6.849
^{189}Os	16.100	188.958	3/2	23.305
^{191}Ir	37.300	190.961	3/2	5.156
^{193}Ir	62.700	192.963	3/2	5.615
^{195}Pt	33.800	194.965	1/2	64.414
^{197}Au	100.000	196.966	3/2	5.189
^{199}Hg	16.840	198.968	1/2	53.756
^{201}Hg	13.220	200.970	3/2	19.845
^{203}Tl	29.500	202.972	1/2	171.746
^{205}Tl	70.500	204.974	1/2	173.433
^{207}Pb	22.600	206.976	1/2	62.601
^{209}Bi	100.000	208.980	9/2	48.228
^{235}U	0.720	235.044	7/2	5.372
electron		0.000	1/2	197000.000

INFRARED ABSORPTION FREQUENCIES FOR SOME INORGANIC SPECIES.

Species	ν/cm^{-1}
NO_3^-	1305 - 1420
SO_4^{2-}	1070 – 1130 and 613
ClO_4^-	1050 - 1170
PO_4^{3-}	1030 - 1100
CN^-	2000 – 2270 (free 2080)
CrO_4^{2-}	840 - 900
MnO_4^-	770 - 810
BF_4^-	1040 - 1100
PF_6^-	800 - 880
NH_4^+	3100 – 3330 and 1360 - 1450
UO_2^{2+}	910 - 930
Terminal metal carbonyl, monoanion	2020 – 1750
Terminal metal carbonyl, neutral	2120 – 1820
μ-bridging metal carbonyl, neutral	1740 - 1880

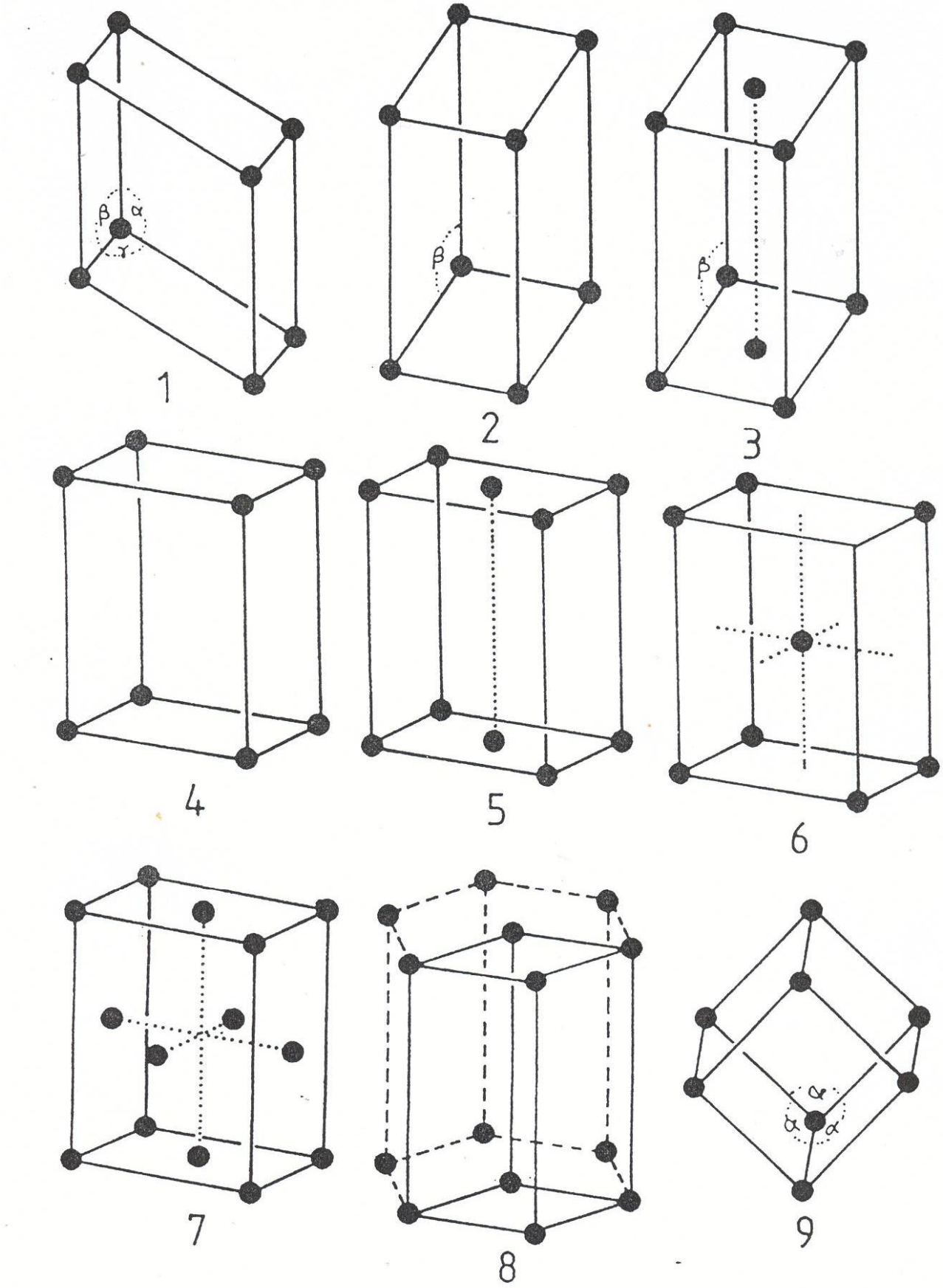
INFRARED ABSORPTION FREQUENCIES
for some Organic Functions

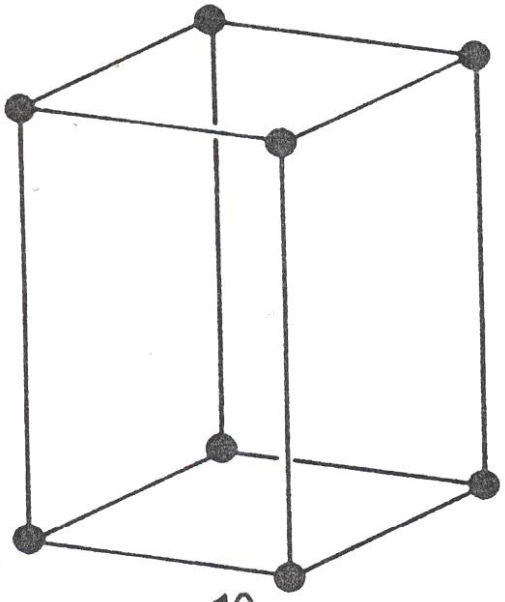
Vibration type	Molecule/Group		υ/cm^{-1}
C–H stretch	Alkyl group	(CH_3, CH_2, CH)	2960 - 2850
	Alkanal	(CHO)	2900 - 2700
	Arene		3040 - 3010
	Alkene	($C=CH_2$)	3095 - 3075
	Alkyne	(C+CH)	3300 - 3270
C–H bend	Alkyl group	(CH_3, CH_2, CH)	1460 - 1370
	Alkene	($C=CH_2$)	990 - 890
	Arene (in-plane)		1300 - 1000
	(out-of-plane)		900 - 650
C–O stretch	Alkanol	(OH)	1200 - 1050
	Alkanoate ester	(C–O)	1300 - 1050
	Alkoxy (ether)	(R_2O)	1150 - 1070
C=O stretch	Alkanal	(RCHO)	1740 - 1720
	Alkanoate ester	(C=O)	1750 - 1730
	Alkanoic acid	(RCO_2H)	1725 - 1700
	Alkanoamide	($RCONR_2$)	1700 - 1630
	Alkanone	(R_2CO)	1740 - 1700
	Alkanoyl chloride	(RCOCl)	1815 - 1790
	Aromatic ketone	(Ar_2CO)	1700 - 1680
C≡N stretch	nitrile	(RCN)	2260 - 2200
N=O stretch	nitro	(NO_2)	1570 - 1510
		and	1370 - 1300
S=O stretch	sulphonate ester	($–SO_3–$)	1420 - 1330
		and	1200 - 1145
M–H stretch	metal-hydride complexes		2200 - 1600
N–H stretch	Amine, amide	(NH_2)	3500 - 3300
O–H stretch	Alkanol	(OH)	3650 - 3590
S–H stretch	Thiol	(SH)	2600 - 2550

Note: Substituents and hydrogen-bonding effects may cause significant variation in the values quoted above; peaks may also show fine structure.

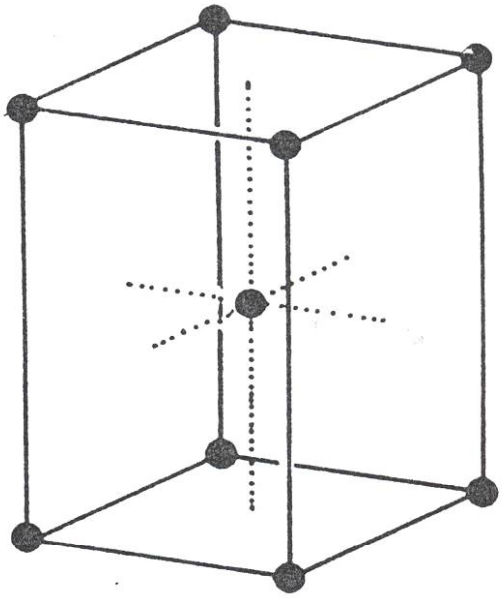
NOTE: Lengths of $a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90^{o}$

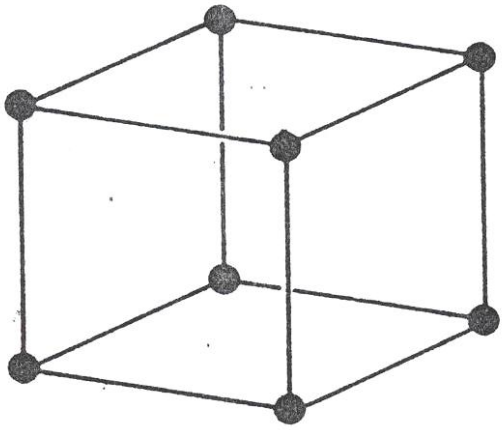




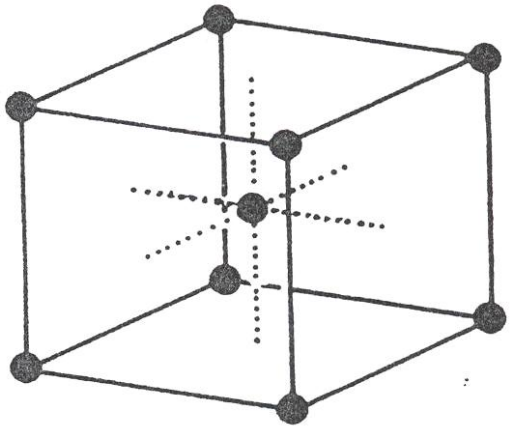
10



11



12



13

The Bravais lattices.

1, Triclinic (P).

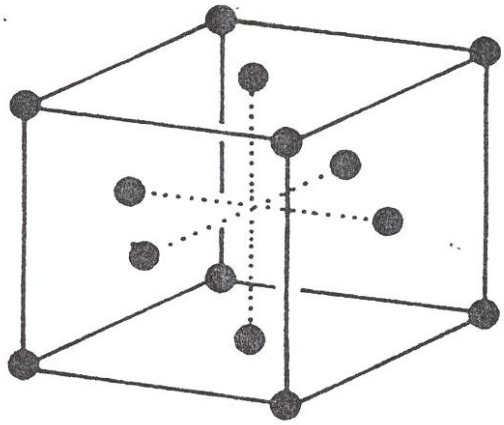
2–3, Monoclinic (P, C),

4–7, Orthorhombic (P, C, I, F).

8, Hexagonal (P). 9, Rhombohedral (R

10–11, Tetragonal (P, I).

12–14, Cubic (P, I, F).



14

PHYSICAL PROPERTIES OF GASES*

	Boiling Point T_b/K	Density ρ/kg m^{-3}	Specific heat capacity at constant pressure C_p/J kg^{-1} K^{-1}	Ratio of specific heats, at 293K, $\gamma = C_p/C_v$	Viscosity at 293 K, 10^6 η/N s m^{-2}	Critical temperature T_c/K	Critical Pressure, P_c/MPa (or MN m^{-2})
Air	83	1.293	993	1.40	17	132	3.77
Ammonia	240	0.771	2190	1.31	9	405	11.3
Argon	87	1.784	524	1.67	21	151	4.86
Carbon dioxide	195	1.977	834	1.30	14	304	7.37
Carbon monoxide	81	1.250	1050	1.40	17	134	3.50
Chlorine	238	3.214	478	1.36	13	417	7.70
Dinitrogen oxide	183	1.978	892	1.30	13	310	7.24
Ethane	185	1.357	1615	1.22	9	305	4.90
Ethene	170	1.260	1500	1.26	10	283	5.12
Ethyne	189	1.173	1590	1.26	9	309	6.20
Helium	4.3	0.179	5240	1.66	19	5.3	0.23
Hydrogen	20.4	0.090	14200	1.41	8	33	1.29
Hydrogen chloride	189	1.640	796	1.40	14	325	8.26
Hydrogen sulfide	211	1.538	1020	1.32	12	374	9.00
Methane	109	0.717	2200	1.31	10	191	4.62
Nitrogen	77	1.250	1040	1.40	17	126	3.38
Nitrogen oxide	121	1.340	972	1.39	18	179	6.5
Nitrogen dioxide	294	1.867	680	1.31	13 (300 K)	431	10.1
Oxygen	90	1.429	013	1.40	19	154	5.1
Sulfur dioxide	263	2.927	645	1.29	9	430	7.9
Water vapour	373	0.600**	2020 **		12 **	647	22.12

* at 273 K and 1 atmosphere pressure unless indicated otherwise ** (373 K)

PHYSICAL PROPERTIES OF LIQUIDS

	Melting Point T_m/K	Boiling Point T_b/K	Density** ρ/kg m^{-3}	Specific latent heat of vaporisation* $10^{-3}\ell$/J kg^{-1}	Specific heat capacity C_p/J kg^{-1} K^{-1}	Cubic Expansivity 10^{-5} γ/ K^{-1}	Viscosity, ** η/ 10^{-3}N s m^{-2}
Benzene	279	353	879	394	1700	122	0.65
Bromine	266	352	3100	183	460	113	0.99
Carbon disulfide	162	319	1293	352	1000	119	0.38
Ethanoic acid	290	391	1049	394	1960	107	1.22
Ethanol	156	352	789	839	2500	108	1.20
Ethoxyethane	157	308	714	372	2300	163	0.24
Mercury	234	630	13546	290	140	18.2	1.55
Methanol	179	338	791	1103	2500	119	0.59
Methylbenzene	178	384	867	350	1670	107	0.58
Nitrobenzene	279	484	1175	330	1400	86	2.03
Phenylamine	267	457	1022				4.4
Propane-1, 2,3-triol	293	563+	1261	830	2400	47	1495
Propanone	178	329	790	522	2210	143	0.32
Tetrachloromethane	250	350	1594	195	840	122	0.97
Trichloromethane	210	335	1483	249	960	127	0.57
Water	273	373	998	2260	4190	21	1.00

* At the boiling point, T_b ** At 293 K + decomposes at this temperature

BLANK

SELECTED PHYSICAL PROPERTIES OF SOME SOLID MATERIALS

	Melting Point T_m/K	**Density 10^{-3} ρ/kg m^{-3}**	**Specific latent heat of fusion 10^{-4} ℓ/J kg^{-1}**	**Specific heat capacity 10^{-2} C_p/J kg^{-1} K^{-1}**	**Linear expansivity 10^5 α/J K^{-1}**	**Thermal conductivity λ/W m^{-1} K^{-1}**
Alumina	2300	3.8	40	8.0	9	30
Aluminium	930	2.7		9.0	23	220
Brass (70Cu/30Zn)	1300	8.5		3.7	18	110
Brick (building)		2.3			9	0.6
" (firebrick)		2.1			5	0.8
Bronze (90Cu/10Sn)	1300	8.8		3.6	17	180
Carbon (graphite)	3700	2.3		7.1	8	5.0
Concrete		2.4		3.4	12	0.1
Constantan (60Cu/40Ni)	1360	8.9		4.2	17	23
Copper	1356	8.9	20	3.9	17	390
Epoxy resin		1.2		14	40	
Fluon		2.2		10	50	0.3
Glass (pyrex-type)	1100*	2.2		~6	3	~1.0
Gold	1340	19.3	7	1.3	14	300
Ice	273	0.9	33	21	50	2.0
Invar (64 Fe/36Ni)	1800	8.0		5	1	
Iron	1810	7.9	27	1.1	12	80
" (cast)	~1450	~7.5	~12		11	75

Lead	600	11.3	3	1.3	30	35
Manganin (83Cu/15Mn/3Ni)		8.5	40	4	18	22
Monel (70Ni/30Cu)	1600	8.8			14	21
Nickel	1726	8.9	30	4.6	13	60
Nylon	470	1.2		17	100	0.3
Perspex	350	1.2		15	85	0.2
Platinum	2042	21.5	11	1.4	9	70
Polyethylene	410	0.9		23	250	
Polypropylene	450	0.9		21	65	
Polystyrene	510	1.1		13	70	0.1
PVC (hard)	485	1.7		10	60	
PVC (soft)	485	1.3		18	150	
Sulfur	386	2.1		7	64	0.3
Sodium	370	0.97	11	12	71	134
Stainless Steel (18Cr/8Ni)	~1800	~8.0		~5	16	150
Steel (mild)	~1700	~8.0		~4	15	60
Titanium	1950	4.5	32	5.2	9	23

* Softening temperature

MOHS' HARDNESS SCALES

The original and modified scales have ten and fifteen points respectively. The points on the original scale are shown in parentheses in the table

Substance	Hardness	Substance	Hardness
Talc	1(1)	Topaz	9(8)
Gypsum	2(2)	(Corundum)	(9)
Calcite	3(3)	Garnet	10
Fluorite	4(4)	Fused zirconia	11
Apatite	5(5)	Fused alumina	12
Orthoclase	6(6)	Silicon carbide	13
Vitreous silica	7	Boron carbide	14
Quartz	8(7)	Diamond	15(10)

STOKES'S LAW OF VISCOSITY

$$v = 2gr^2 (\rho - \rho_O)/(9\eta)$$

where

- v is the terminal velocity of fall of a spherical particle in a viscous medium
- r is the radius of the particle
- ρ is the density of the particle
- ρ_O is the density of the medium
- η is the coefficient of viscosity of the medium

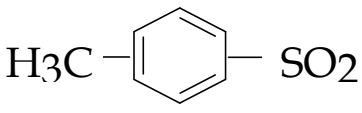
SELECTED STABILITY CONSTANTS

Chemistry Data Book 2nd edition J G Stark, H G Wallace, John Murray Ltd, London, 1982.

Log_{10} (Stability Constants of Complex Ions at 298 K)

Ag^{+}	+	$2NH_3$	=	$[Ag(NH_3)_2]^{+}$	7.22
Co^{3+}	+	$6NH_3$	=	$[Co(NH_3)_6]^{3+}$	23.12
Cu^{2+}	+	$4NH_3$	=	$[Cu(NH_3)_4]^{2+}$	12.36
Zn^{2+}	+	$4NH_3$	=	$[Zn(NH_3)_4]^{2+}$	8.56
Ag^{+}	+	$2CN^{-}$	=	$[Ag(CN)_2]^{-}$	20.4
Fe^{3+}	+	$6CN^{-}$	=	$[Fe(CN)_6]^{3-}$	52.61
Cu^{+}	+	$4CN^{-}$	=	$[Cu(CN)_4]^{3--}$	33.02
Zn^{2+}	+	$4CN^{-}$	=	$[Zn(CN)_4]^{2-}$	16.76
Ag^{+}	+	$EDTA^{4-}$	=	$[Ag(EDTA)]^{3-}$	7.3
Ca^{2+}	+	$EDTA^{4-}$	=	$[Ca(EDTA)]^{2-}$	10.7
Co^{2+}	+	$EDTA^{4-}$	=	$[Co(EDTA)]^{2-}$	16.2
Co^{3+}	+	$EDTA^{4-}$	=	$[Co(EDTA)]^{-}$	36
Cu^{2+}	+	$EDTA^{4-}$	=	$[Cu(EDTA)]^{2-}$	18.8
Fe^{3+}	+	$EDTA^{4-}$	=	$[Fe(EDTA)]^{-}$	25.7
Fe^{2+}	+	$EDTA^{4-}$	=	$[Fe(EDTA)]^{2-}$	14.3
Mg^{2+}	+	$EDTA^{4-}$	=	$[Mg(EDTA)]^{2-}$	8.7
Zn^{2+}	+	$EDTA^{4-}$	=	$[Zn(EDTA)]^{2-}$	16.5

COMMON ABBREVIATIONS

Ar	any aryl group
Bn	benzyl $C_6H_5CH_2$-
BOC	$CO_2{}^tBu$
Bz	benzoyl C_6H_5-CO-
CBZ (Z)	CO_2Bn
LDA	Lithium diisopropylamide
MCPBA	meta-chloroperbenzoic acid ($3\text{-}ClC_6H_4CO_3H$)
PCC	pyridinium chlorochromate $(C_5H_5\overset{+}{N}H \quad ClCrO_3^-)$
R	any alkyl group
TBDMS (TBS)	$\text{-}SiMe_2{}^tBu$
Tf	triflate -OSO_2CF_3
TFA	trifluoroacetic acid, CF_3CO_2H
THF	Tetrahydrofuran
THP	tetrahydropyran
TMS	-trimethylsilyl -$SiMe_3$ or tetramethylilane Me_4Si (in context of NMR)
Ts	tosyl 

BRIEF SUMMARY OF ORGANIC NOMENCLATURE ACCORDING TO THE IUPAC SYSTEM

The nomenclature of organic compounds can be very complex but most common compounds can be named using a few simple rules. The principal part of the structure will be a chain or a cyclic system. If there are several possible chains the longest one is chosen. If possible the most important functional group (that is whichever group appears highest in Table A) should be included in the principal part. Many functional groups can be named either as prefixes or as suffixes (see Table A). If any group at all is present which can be named as a suffix, then there must be a suffix in the name. If several such groups are present, then the most important group is the one to be named as suffix the other groups being named as prefixes

e.g $CH_3CO(CH_2)_3CO_2H$ is 5-oxohexanoic acid, but

$CH_3CO(CH_2)_4OH$ is 6-hydroxyhexan-2-one.

However the suffixes -ene and -yne can be compounded with suffixes denoting another group as the principal group, e.g., cyclohex-2-enone (note the terminal e in ene is omitted in such cases).

Numbers (locants) normally have to be used to denote the position of each group. The numbering is such as to give the major group the lowest possible number. Where there is no ambiguity a number is not used. For instance an -oic acid has to be at the end of the chain and hence (usually) at position 1.

The groups listed in Table B can be named only as prefixes. If there is more than one group prefixing the name of the principal part of the structure these are placed in alphabetical order, each one preceded by the appropriate locant. If several groups are the same they are not repeated as separate prefixes but the Greek numerical term is used instead to show how many there are

e.g 2,3,3-trimethylcyclopentanone

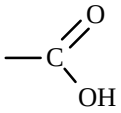
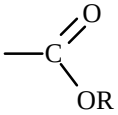
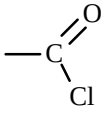
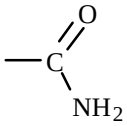
Finally many heterocyclic systems have individual names. The major ones are listed on the Structures of Selected Heterocyclic Organic Compounds' table.

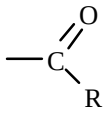
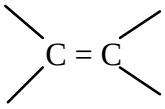
For use when naming compounds

TABLE A

ORDER OF PRECEDENCE FOR COMMON GROUPS

(highest precedence at the top)

Group	Suffix	Prefix
	–ammonium	----
	–oic acid* –carboxylic acid†	carboxy–
	alkyl –oate* alkyl carboxylate†	alkoxycarbonyl–
–SO_3H	–sulfonic acid	sulfo–
	–oyl chloride* –carbonyl chloride†	chlorocarbonyl–
	–amide* –carboamide†	carbamoyl–
–CHO	-al* -carbaldehyde†	oxo–* methanoyl-†

Group	Suffix	Prefix
	-one	oxo-* alkanoyl-†
–**C** ≡ N	–onitrile* –carbonitrile†	cyano–
–OH	–ol	hydroxy–
–SH	–thiol	mercapto–
–NH_2	–amine	amino–
–NH(COR)	–amide	amido–
	-ene	
–C ≡ C–	–yne	

* Term used if part of a chain (note the carbon atom counts as part of the chain)

† Term used if substituent is on, e.g., a ring

TABLE B

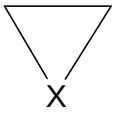
SUBSTITUENTS NAMED ONLY AS PREFIXES

Group	Prefix
–OR	alkoxy-
–SR	alkylthio-
–SO–	sulfinyl-
$–SO_2–$	sulfonyl-
–H (added)	hydro -
–F, Cl, Br, I	halogeno-
–NO	nitroso-
$–NO_2$	nitro-
–N=N–	azo-
–O–O–	peroxo

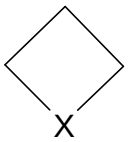
In addition, hydrocarbon and heterocyclic groups are named as prefixes (methyl, phenyl, cyclohexyl, indol-3-yl) unless they are chosen as the principal part of the structure.

STRUCTURES OF SELECTED CYCLIC ORGANIC COMPOUNDS

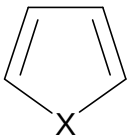
Acridine	(39)			
Anthracene	(38)		Oxazole	(12)
Azepine	(21)		Oxepine	(22)
Azetidine	(3)		Oxetane	(4)
Aziridine	(1)		Oxirane (an epoxide)	(2)
Azulene	(27)		Phenanthrene	(40)
Benzofuran	(28)		Phenanthridine	(41)
Benzothiophen	(30)		Piperidine	(14)
Carbazole	(36)		Purine	(26)
β-Carboline	(37)		2H-Pyran	(20)
Dioxan	(16)		Pyrazole	(8)
Furan	(6)		Pyridine	(17)
Imidazole	(11)		Pyrylium	(18)
Indole	(29)		Pyrimidine	(19)
Indolizine	(25)		Pyrrole	(5)
Isoindole	(24)		Quinazoline	(35)
Isoquinoline	(33)		Quinoline	(32)
Isothiazole	(10)		Quinoxaline	(34)
Isoxazole	(9)		Thiazole	(13)
Morpholine	(15)		Thiophene	(7)
Naphthalene	(31)		Tropylium	(23)



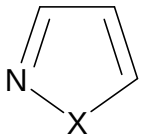
(1) X = NH
(2) X = O



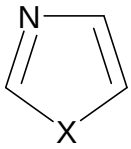
(3) X = NH
(4) X = O



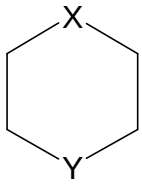
(5) X = NH
(6) X = O
(7) X = S



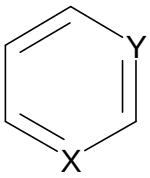
(8) X = NH
(9) X = O
(10) X = S



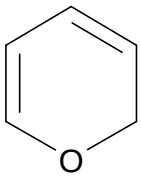
(11) X = NH
(12) X = O
(13) X = S



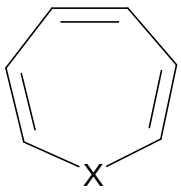
(14) X = NH, Y = CH_2
(15) X = NH, Y = O
(16) X = Y = O



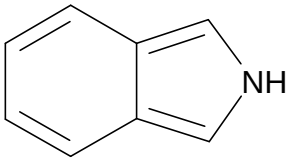
(17) X = N, Y = CH
(18) X = O^+, Y = CH
(19) X = Y = N



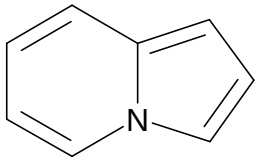
(20)



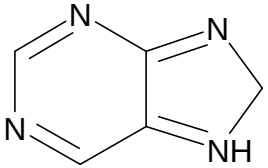
(21) X = NH
(22) X = O
(23) X = CH^+



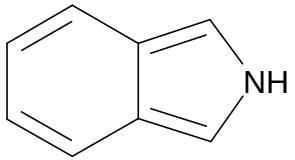
(24)



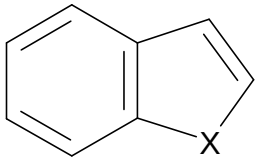
(25)



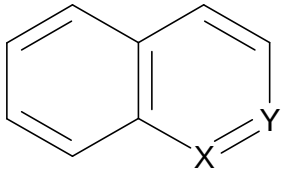
(26)



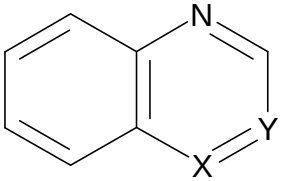
(27)



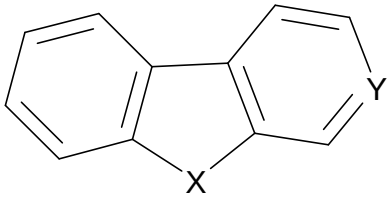
(28) X = O
(29) X = NH
(30) X = S



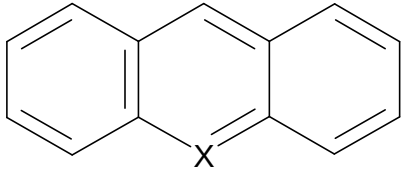
(31) X = Y = CH
(32) X = N, Y = CH
(33) X = CH, Y = N



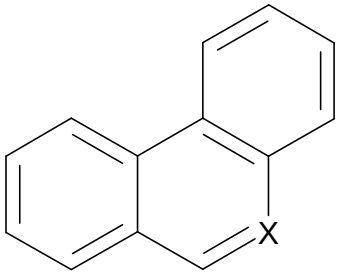
(34) X = N, Y = CH
(35) X = CH, Y = N



(36) X = NH, Y = CH
(37) X = NH, Y = N

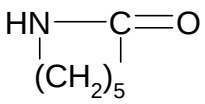
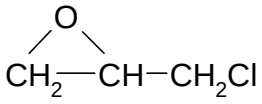
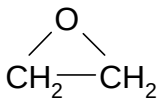


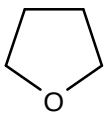
(38) X = CH
(39) X = N



(40) X = CH
(41) X = N

STRUCTURES OF SELECTED ORGANIC COMPOUNDS FREQUENTLY REFERRED TO BY NON-SYSTEMATIC NAMES
(standard abbreviations shown in brackets)

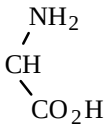
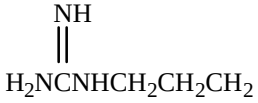
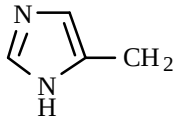
Acetic Acid		$MeCO_2H$
Acetone		MeCOMe
Acetylene		CH≡CH
Acrolein		CH_2=CHCHO
Acrylic Acid		CH_2=$CHCO_2H$
Acrylonitrile		CH_2=CHCN
Adipic Acid		$HO_2C(CH_2)_4CO_2H$
Aniline		$PhNH_2$
Bisphenol A		$(4\text{-}HOC_6H_4)_2CMe_2$
Chloroform		$CHCl_3$
Chloroprene		CH_2=$CClCH$=CH_2
Cresol		MeC_6H_4OH
Cumene		$PhCHMe_2$
Dimethylformamide	(DMF)	Me_2NCHO
Dimethylsulfoxide	(DMSO)	Me_2SO
ε-Caprolactam		
Epichlorohydrin		
Ethylene Glycol		$HOCH_2CH_2OH$
Ethylene Oxide		
		continued

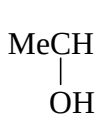
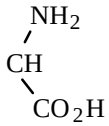
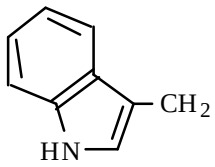
Formaldehyde		CH_2O
Formic Acid		HCO_2H
Glycerol		$HOCH_2CH(OH)CH_2OH$
Hexamethylenediamine		$H_2N(CH_2)_6NH_2$
Iso-octane		$Me_3CCH_2CHMe_2$
Isobutylene		$Me_2C=CH_2$
Ketene		$CH_2=C=O$
Methylene Dichloride		CH_2Cl_2
Methyl Methacrylate		$CH_2=CMeCO_2Me$
Neoprene		$[-CH_2CCl=CHCH_2-]_n$
Oxalic Acid		$HO_2C.CO_2H$
Phosgene		Cl_2CO
Phthalic Acid		$1,2\text{-}C_6H_4(CO_2H)_2$
Propylene		$MeCH=CH_2$
PVC		$[-CH_2CHCl-]_n$
Stilbene		$PhCH=CHPh$
Styrene		$PhCH=CH_2$
Succinic Acid		$HO_2CCH_2CH_2CO_2H$
Terephthalic Acid		$1,4\text{-}C_6H_4(CO_2H)_2$
Tetrahydrofuran	(THF)	
Toluene		PhMe
Urea		H_2NCONH_2
Vinyl Chloride		$CH_2=CHCl$
Xylene		$C_6H_4Me_2$

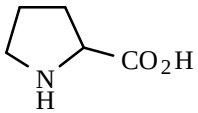
NON-SYSTEMATIC NAMES AND STRUCTURES OF SELECTED ORGANIC GROUPS
(standard abbreviations shown in parentheses)

Amyl		$CH_3(CH_2)_4–$
i-Amyl (Isoamyl)		$(CH_3)_2CH(CH_2)_2–$
Butyl	(Bu)	$CH_3(CH_2)_3–$
i-Butyl (Isobutyl)	(Bu^i)	$(CH_3)_2CHCH_2–$
s-Butyl	(Bu^s)	$CH_2CH_2CHCH_3$ |
t-Butyl	(Bu^t)	$(CH_3)_3C–$
Ethyl	(Et)	$CH_3CH_2–$
Methyl	(Me)	$CH_3–$
Neopentyl		$(CH_3)_3CCH_2–$
Propyl	(Pr)	$CH_3CH_2CH_2–$
i-Propyl (Isopropyl)	(Pr^i)	$(CH_3)_2CH–$
Allyl		$CH_2=CHCH_2–$
Benzyl	(Bn)	$C_6H_5CH_2–$
Benzylidene		$C_6H_5CH=$
Ethylidene		$CH_3CH=$
Phenyl	(Ph)	$C_6H_5–$
Propargyl		$HC\equiv CCH_2–$
Vinyl		$CH_2=CH–$
Acetate	(AcO)	$CH_3CO_2–$
Acetyl	(Ac)	$CH_3CO–$
Acrylate		$CH_2=CHCO_2–$
Benzoyl	(Bz)	$C_6H_5CO–$
Brosylate	(Bs)	$4\text{-}BrC_6H_4SO_3–$
Mesylate	(Ms)	$CH_3SO_3–$
Methacrylate		$CH_2=C(CH_3)CO_2–$
Phenacyl		$C_6H_5COCH_2–$
Tosylate	(Ts)	$4\text{-}CH_3C_6H_4SO_3–$
Triflate	(Tf)	$CF_3SO_3–$
Trityl		$(C_6H_5)_3C\text{-}$

AMINO ACIDS

Name	**Single Letter code**			**Common Structure**
alanine (Ala)	A	Me	--	
arginine (Arg)	R		--	
aspartic acid (Asp)	D	HO_2CCH_2	--	
asparagine (Asn)	N	H_2NCOCH_2	--	
cysteine (Cys)	C	$HSCH_2$	--	
glutamic acid (Glu)	E	$HO_2CCH_2CH_2$	--	
glutamine (Gln)	Q	$H_2NCOCH_2CH_2$	--	
glycine (Gly)	G	H	--	
histidine (His)	H		--	
isoleucine (Ile)	I		--	
leucine (Leu)	L	Me_2CHCH_2	--	
lysine (Lys)	K	$H_2NCH_2CH_2CH_2CH_2$	--	
methionione (Met)	M	$MeSCH_2CH_2$	--	
phenylalanine (Phe)	F	$PhCH_2$	--	
serine (Ser)	S	$HOCH_2$	--	

Name	**Single Letter code**			**Common Structure**
threonine (Thr)	T		--	
tryptophan (Trp)	W		--	
tyrosine (Tyr)	Y	4-HOC6H4CH2	--	
valine (Val)	V	Me2CH	--	

proline (Pro)	P	 *full structure shown*	

THE GENETIC CODE (RELATING BASE SEQUENCE IN DNA TO AMINO-ACID SEQUENCE IN PROTEIN)

First Position (5′end)	Second Position				Third Position (3′end)
	U	**C**	**A**	**G**	
	Phe	Ser	Tyr	Cys	**U**
	Phe	Ser	Tyr	Cys	**C**
U	Leu	Ser	Stop	Stop	**A**
	Leu	Ser	Stop	Trp	**G**
	Leu	Pro	His	Arg	**U**
	Leu	Pro	His	Arg	**C**
C	Leu	Pro	Gln	Arg	**A**
	Leu	Pro	Gln	Arg	**G**
	lle	Thr	Asn	Ser	**U**
	lle	Thr	Asn	Ser	**C**
A	lle	Thr	Lys	Arg	**A**
	Met	Thr	Lys	Arg	**G**
	Val	Ala	Asp	Gly	**U**
	Val	Ala	Asp	Gly	**C**
G	Val	Ala	Glu	Gly	**A**
	Val	Ala	Glu	Gly	**G**

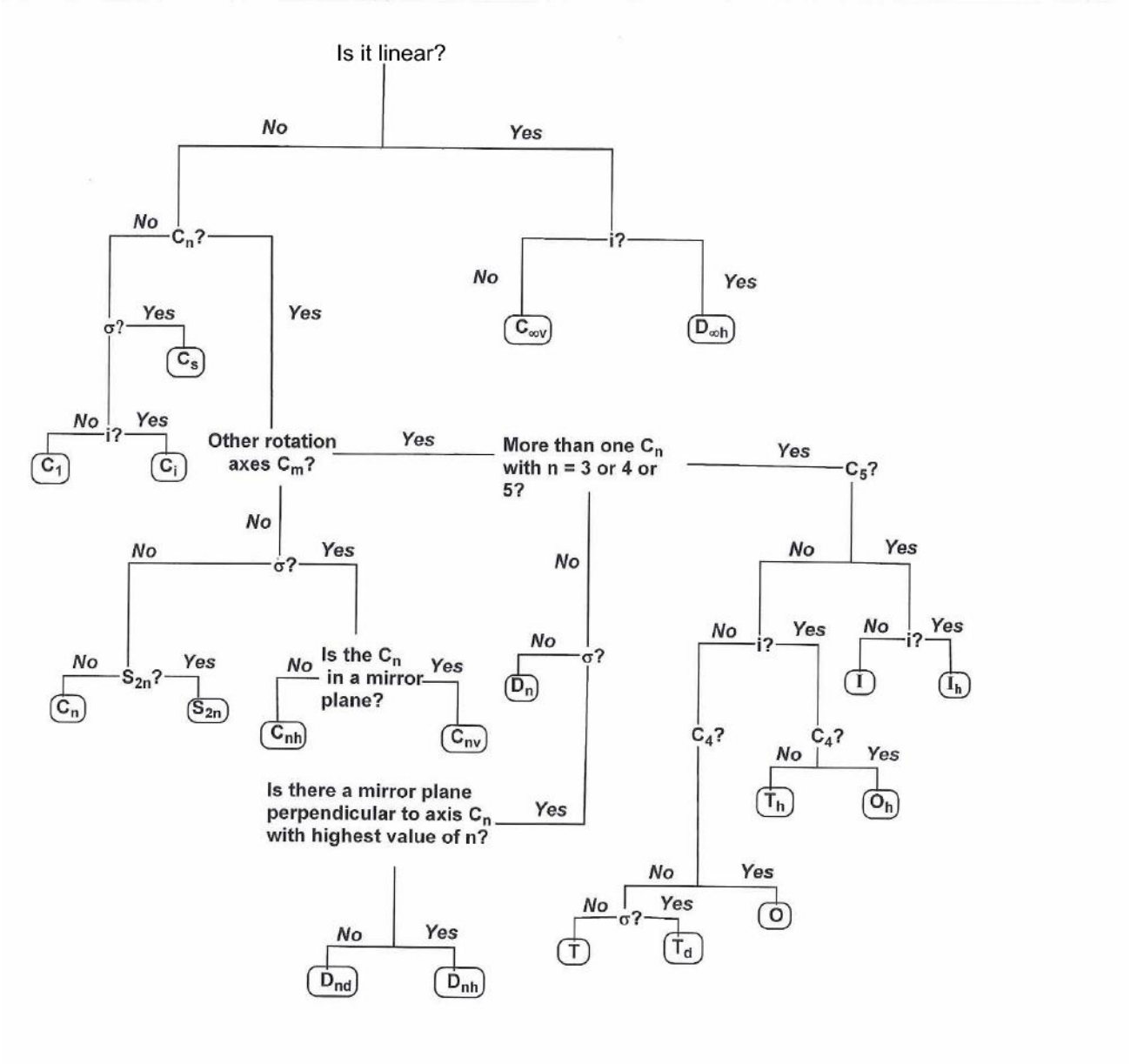
APPROXIMATE pK_A VALUES OF SELECTED ORGANIC COMPOUNDS

Acid	Base	pK_a
$PhSO_3H$	$PhSO_3^-$	–7
RCO_2H	RCO_2^-	4 - 5
PhOH	PhO^-	10
$RCOCH_2CO_2R$	$RCO\bar{C}HCO_2R$	11
RCH_2OH	RCH_2O^-	16
RCH_2COR	$R\bar{C}HCOR$	19
RCH_2CO_2R	$R\bar{C}HCO_2R$	25
$RC\equiv CH$	$RC\equiv C^-$	25
$R_2C\text{-}CH_2$	$R_2C=\bar{C}H$	44
RCH_3	$R\bar{C}H_2$	50

SELECTED HAMMETT SUBSTITUTENT CONSTANTS

Substituent	σ_m	σ_p	σ_p^+	σ_p^-	σ_p^o
$-NO_2$	0.71	0.78	0.78	1.24	0.82
$-C\equiv N$	0.61	0.70	0.70	0.88	0.71
-C(O)Me	0.38	0.50	0.50	0.84	0.46
$-CO_2R$	0.32	0.45	0.45	0.64	0.44
$-CF_3$	0.43	0.54	0.54	0.65	0.53
-I	0.35	0.28	0.14	0.28	0.27
-Br	0.39	0.23	0.15	0.23	0.26
-Cl	0.37	0.22	0.11	0.22	0.27
-F	0.34	0.06	-0.07	0.06	0.17
-OMe	0.11	-0.28	-0.78	-0.28	-0.12
-Ph	0.05	0.00	-0.21	0.08	0.05
-H	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
-Me	-0.07	-0.17	-0.31	-0.17	-0.07
$-NH_2$	-0.16	-0.66	-1.30	-0.66	-0.38
$-NMe_2$	-0.15	-0.63	-1.70	-0.63	-0.32

HOW TO ASSIGN A MOLECULE TO ITS POINTS GROUP



SELECTED CHARACTER TABLES FOR CHEMICALLY IMPORTANT GROUPS

1 The Non-axial Groups

C_s	E	σ_h		
A′	1	1	x, y, R_z	x^2, y^2, z^2, xy
A″	1	–1	z, R_x, R_y	yz, xz

C_i	E	i		
A_g	1	1	R_x, R_y, R_z	x^2, y^2, z^2, xy, yz, xz
A_u	1	–1	x, y, z,	

2 The C_n Groups

C_2	E	C_2		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	–1	x, y, R_x, R_y	yz, xz

3 The D_n Groups

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	–1	–1	z, R_z	xy
B_2	1	–1	1	–1	y, R_y	xz
B_3	1	–1	–1	1	x, R_x	yz

D_3	E	$2C_3$	$3\,C_2$		
A_1	1	1	1		$x^2 + y^2$, z^2
A_2	1	1	–1	z, R_z	
E	2	–1	0	(x,y)(R_x, R_y)	(x^2–y^2,xy)(xz,yz)

4 The C_{nv} Groups

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$			
A_1	1	1	1	1	z	x^2, y^2, z^2	z^3, x^2z, y^2z
A_2	1	1	–1	–1	R_z	xy	xyz
B_1	1	–1	1	–1	x, R_y	xz	xz^2, x^3, xy^2
B_2	1	–1	–1	1	y, R_x	yz	yz^2, y^3, x^2y

C_{3v}	E	$2C_3$	$3\sigma_v$			
A_1	1	1	1	z	$x^2 + y^2$, z^2	z^3,$x(x^2-3y^2)$, z $(x^2 + y^2)$
A_2	1	1	–1	R_z		$y(3x^2 – y^2)$
E	2	–1	0	(x,y) (R_x,R_y)	$(x^2-y^2,xy)(xz,yz)$	$(xz^2,yz^2)[xyz, z(x^2 –y^2)][x(x^2+y^2), y(x^2+y^2)]$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 + y^2$, z^2
A_2	1	1	1	–1	–1	R_z	
B_1	1	–1	1	1	–1		$x^2 – y^2$
B_2	1	–1	1	–1	1		xy
E	2	0	–2	0	0	(x,y)(R_x,R_y)	(xz,yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	R_z	
E_1	2	$2 \cos 72^o$	$2 \cos 144^o$	0	$(x,y)(R_x,R_y)$	(xz,yz)
E_2	2	$2 \cos 144^o$	$2 \cos 72^o$	0		$x^2 - y^2$, xy

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	–1	–1	R_z	
B_1	1	–1	1	–1	1	–1		
B_2	1	–1	1	–1	–1	1		
E_1	2	1	–1	–2	0	0	$(x,y)(R_x,R_y)$	(xy,yz)
E_2	2	–1	–1	2	0	0		$x^2 - y^2$, xy

5 The C_{nh} Groups

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	–1	1	–1	R_x,R_y	(xz,yz)
A_u	1	1	–1	–1	z	
B_u	1	–1	–1	1	x,y	

6 The D_{nh} Groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	σ(xy)	σ(xz)	σ(yz)		
A_g	1	1	1	1	1	1	1	1		x^2,y^2,z^2
B_{1g}	1	1	–1	–1	1	1	–1	–1	R_z	xy
B_{2g}	1	–1	1	–1	1	–1	1	–1	R_y	xz
B_{3g}	1	–1	–1	1	1	–1	–1	1	R_x	yz
Au	1	1	1	1	–1	–1	–1	–1		
B_{1u}	1	1	–1	–1	–1	–1	1	1	z	
B_{2u}	1	–1	1	–1	–1	1	–1	1	y	
B_{3u}	1	–1	–1	1	–1	1	1	-1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A'_1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A'_2	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x,y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x,R_y)	(xz, yz)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$			
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$	
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z		
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		$x^2 - y^2$	
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy	
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz,yz)	
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1			
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z		$z^3, z(x^2+y^2)$
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1			xyz
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1			$z(x^2 - y^2)$
E_u	2	0	-2	0	0	-2	0	2	0	0	(x, y)		$(xz^2,yz^2)(xy^2,x^2y)$ (x^3, y^3)

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2'$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
A_1'	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	1	–1	1	1	1	–1	R_z	
E_1'	2	$2\cos 72^o$	$2\cos 144^o$	0	2	$2\cos 72^o$	$2\cos 144^o$	0	(x, y)	
E_2'	2	$2\cos 144^o$	$2\cos 72^o$	0	2	$2\cos 144^o$	$2\cos 72^o$	0		$(x^2 - y^2, xy)$
A_1''	1	1	1	1	–1	–1	–1	–1		
A_2''	1	1	1	–1	–1	–1	–1	1	z	
E_1''	2	$2\cos 72^o$	$2\cos 144^o$	0	–2	$-2\cos 72^o$	$-2\cos 144^o$	0	(R_x, R_y)	(xy, yz)
E_2''	2	$2\cos 144^o$	$2\cos 72^o$	0	–2	$-2\cos 144^o$	$-2\cos 72^o$	0		

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	1	–1	–1	1	1	1	1	–1	–1	R_z	
B_{1g}	1	–1	1	–1	1	–1	1	-1	1	–1	1	–1		
B_{2g}	1	–1	1	–1	–1	1	1	–1	1	–1	–1	1		
E_{1g}	2	1	–1	–2	0	0	2	1	–1	–2	0	0	(R_x,R_y)	(xz,yz)
E_{2g}	2	–1	–1	2	0	0	2	–1	–1	2	0	0		(x^2-y^2, xy)
A_{1u}	1	1	1	1	1	1	–1	–1	–1	–1	–1	–1		
A_{2u}	1	1	1	1	–1	–1	–1	–1	–1	–1	1	1	z	
B_{1u}	1	–1	1	–1	1	–1	–1	1	–1	1	–1	1		
B_{2u}	1	–1	1	–1	–1	1	–1	1	–1	1	1	–1		
E_{1u}	2	1	–1	–2	0	0	–2	–1	1	2	0	0	(x, y)	
E_{2u}	2	–1	–1	2	0	0	–2	1	1	–2	0	0		

7 The D_{nd} Groups

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$			
A_1	1	1	1	1	1		$x^2 + y^2, z^2$	xyz
A_2	1	1	1	–1	–1	R_z		$z(x^2 - y^2)$
B_1	1	–1	1	1	–1		$x^2 - y^2$	
B_2	1	–1	1	–1	1	z	xy	$z^3, z(x^2 + y^2)$
E	2	0	–2	0	0	(x, y) (R_x, R_y)	(xz, yz)	$(xz^2, yz^2)(xy^2, x^2y)(x^3, y^3)$

D_{3d}	E	$2C_3$	$3C_2'$	i	$2S_6$	$3\sigma_d$			
A_{1g}	1	1	1	1	1	1		$x^2 + y^2, z^2$	
A_{2g}	1	1	–1	1	1	–1	R_z		
E_g	2	–1	0	2	–1	0	(R_x, R_y)	$(x^2 - y^2, xy)(xz, yz)$	
A_{1u}	1	1	1	–1	–1	–1			$x(x^2 - 3y^2)$
A_{2u}	1	1	–1	–1	–1	1	z		$y(3x^2 - y^2), z^3, z(x^2 + y^2)$
E_u	2	–1	0	–2	1	0	(x,y)		$(xz^2, yz^2)[xyz, z(x^2 - y^2)]$ $[x(x^2 + y^2), y(x^2 + y^2)]$

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$		
A_1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	1	–1	–1	R_z	
B_1	1	–1	1	–1	1	1	–1		
B_2	1	–1	1	–1	1	–1	1	z	
E_1	2	$2^{½}$	0	$-2^{½}$	–2	0	0	(x, y)	
E_2	2	0	–2	0	2	0	0		$(x^2 - y^2, xy)$
E_3	2	$–2^{½}$	0	$2^{½}$	–2	0	0	(R_x,R_y)	(xz, yz)

D_{5d}	E	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	–1	1	1	1	–1	R_z	
E_{1g}	2	$2\cos 72^o$	$2\cos 144^o$	0	2	$2\cos 72^o$	$2\cos 144^o$	0	$(R_x,\ R_y)$	(xz, yz)
E_{2g}	2	$2\cos 144^o$	$2\cos 72^o$	0	2	$2\cos 144^o$	$2\cos 72^o$	0		$(x^2 - y^2, xy)$
A_{1u}	1	1	1	1	–1	–1	–1	–1		
A_{2u}	1	1	1	–1	–1	–1	–1	1	z	
E_{1u}	2	$2\cos 72^o$	$2\cos144^o$	0	–2	$–2\cos 72^o$	$–2\cos 144^o$	0	(x, y)	
E_{2u}	2	$2\cos 144^o$	$2\cos72^o$	0	–2	$–2\cos 144^o$	$–2\cos 72^o$	0		

8 The Cubic Group

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$			
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$	xyz
A_2	1	1	1	–1	–1			
E	2	–1	2	0	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$	
T_1	3	0	–1	1	–1	(R_x, R_y, R_z)		$[x(z^2 - y^2), y(z^2 - x^2), z(x^2 - y^2)]$
T_2	3	0	–1	–1	1	(x,y,z)	(xy, xz, yz)	$(x^3, y^3, z^3)[x(z^2 + y^2), y(z^2 + x^2), z(x^2 + y^2)]$

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$			
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$	
A_{2g}	1	1	–1	–1	1	1	–1	1	1	–1			
E_g	2	–1	0	0	2	2	0	–1	2	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$	
T_{1g}	3	0	–1	1	–1	3	1	0	–1	–1	(R_x, R_y, R_z)		
T_{2g}	3	0	1	–1	–1	3	–1	0	–1	1		(xz, yz, xy)	
A_{1u}	1	1	1	1	1	–1	–1	–1	–1	–1			
A_{2u}	1	1	–1	–1	1	–1	1	–1	–1	1			xyz
E_u	2	–1	0	0	2	–2	0	1	–2	0			
T_{1u}	3	0	–1	1	–1	–3	–1	0	1	1	(x, y, z)		(x^3, y^3, z^3), $[x(z^2 + y^2), y(z^2 + x^2), z(x^2 + y^2)]$
T_{2u}	3	0	1	–1	–1	–3	1	0	1	–1			$[x(z^2 - y^2), y(z^2 - x^2), z(x^2 - y^2)]$

9 The Continuous Groups

$C_{\infty v}$	**E**	$2C_{\infty}^{\phi}$	. . .	∞ $\boldsymbol{\sigma_v}$		
$\mathbf{A_1} \equiv \sum^+$	**1**	1	. . .	1	z	$x^2 + y^2, z^2$
$\mathbf{A_2} \equiv \sum^-$	**1**	1	. . .	–1	R_Z	
$\mathbf{E_1} \equiv \prod$	2	2cos φ	. . .	0	$(x, y)(R_X, R_Y)$	(xz, yz)
$\mathbf{E_2} \equiv \mathbf{\Delta}$	2	2cos 2φ	. . .	0		$(x^2 - y^2, xy)$
$\mathbf{E_2} \equiv \mathbf{\Phi}$	2	2cos 3φ	. . .	0		
. . .	. . .	. . .	. . .	. . .		

$\mathbf{D_{\infty h}}$	**E**	$2\mathbf{C}_{\infty}^{\phi}$	. . .	$\infty\,\boldsymbol{\sigma}_v$	**i**	$2\mathbf{S}_{\infty}^{\phi}$	. . .	$\infty\mathbf{C}_2'$		
$\mathbf{A_{1g}} \equiv \sum g^+$	1	1	. . .	1	1	1	. . .	1		$x^2 + y^2, z^2$
$\mathbf{A_{2g}} \equiv \sum g^-$	1	1	. . .	–1	1	1	. . .	–1	R_z	
$\mathbf{E_{1g}} \equiv \prod g$	2	2cos φ	. . .	0	2	–2cos φ	. . .	0	(R_x, R_y)	(xz, yz)
$\mathbf{E_{2g}} \equiv \Delta g$	2	2cos 2φ	. . .	0	2	2cos 2φ	. . .	0		$(x^2 - y^2, xy)$
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .		
$\mathbf{A_{1u}} \equiv \sum u^+$	1	1	. . .	1	–1	–1	. . .	–1	z	
$\mathbf{A_{2u}} \equiv \sum u^-$	1	1	. . .	–1	–1	-1	. . .	1		
$\mathbf{E_{1u}} \equiv \prod u$	2	2cos φ	. . .	0	–2	2cos φ	. . .	0	(x, y)	
$\mathbf{E_{2u}} \equiv \Delta u$	2	2cos 2φ	. . .	0	–2	–2cos 2φ	. . .	0		
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .		

GROUP THEORETICAL FORMULAE

Reduction Formula: In more complex cases, it is not always easy to pick out the correct linear combination, in which case we use the *reduction formula:*

$$n(\Gamma) = \frac{1}{h} \sum_{all\,classes} \chi_R \chi_I N$$

$n(\Gamma)$ = number of times a given irreducible representation, Γ, occurs in the sum

χ_R = character in the reducible representation

χ_I = character in the irreducible representation

h = order of the group

N = number of symmetry operations in a given class

Operation	f(R)
E	3
σ	1
i	-3
C_2	-1
C_3	0
C_4	1
C_6	2

Operation	f(R)
S_3	-2
S_4	-1
S_6	0
C_n^k	$1 + 2\cos(2\pi\, k/n)$
s_n^k	$-1 + 2\cos(2\pi\, k/n)$

DIRECT PRODUCT RULES FOR CHEMICALLY IMPORTANT GROUPS

1 General Rules

x	′	″
′	′	″
″	″	′

x	g	u
g	g	u
u	u	g

Unless otherwise indicated (see e.g., table 3)

x	1	2
1	1	2
2	2	1

The antisymmetric component of a product of degenerate components is identified by square brackets [].

2 For C_2, D_3, C_{2v}, C_{3v}, C_{6v}, C_{2h}, D_{3h}, D_{6h}, D_{3d}

x	A_1	A_2	B_1	B_2	E_1	E_2
A_1	A_1	A_2	B_1	B_2	E_1	E_2
A_2		A_1	B_2	B_1	E_1	E_2
B_1			A_1	A_2	E_2	E_1
B_2				A_1	E_2	E_1
E_1					$A_1 + [A_2] + E_2$	$B_1 + B_2 + E_1$
E_2						$A_1 + [A_2] + E_2$

Note symmetry about diagonal

3 For D_2, D_{2h}

x	A	B_1	B_2	B_3
A	A	B_1	B_2	B_3
B_1		A	B_3	B_2
B_2			A	B_1
B_3				A

4 For C_{4v}, C_{4h}, D_{2d}

x	A_1	A_2	B_1	B_2	E
A_1	A_1	A_2	B_1	B_2	E
A_2		A_1	B_2	B_1	E
B_1			A_1	A_2	E
B_2				A_1	E
E					A_1+ [A_2] + B_1 + B_2

5 For C_{5v}, D_{5h}, D_{5d}

x	A_1	A_2	E_1	E_2
A_1	A_1	A_2	E_1	E_2
A_2		A_1	E_1	E_2
E_1			A_1+ [A_2] + E_2	E_1 + E_2
E_2				A_1+ [A_2] + E_1

6 For O_h, T_d

x	A_1	A_2	E	T_1	T_2
A_1	A_1	A_2	E	T_1	T_2
A_2		A_1	E	T_2	T_1
E			$A_1 + [A_2] + E$	$T_1 + T_2$	$T_1 + T_2$
T_1				$A_1 + E + [T_1] + T_2$	$A_2 + E + T_1 + T_2$
T_2					$A_1 + E + [T_1] + T_2$

7 For $C_{\infty v}$, $D_{\infty h}$

x	Σ^+	Σ^-	Π	Δ .....
Σ^+	Σ^+	Σ^-	Π	Δ
Σ^-		Σ^+	Π	Δ
Π			$\Sigma^+ + [\Sigma^-] + \Delta$	$\Pi + \Phi$
Δ				$\Sigma^+ + [\Sigma^-] + \Gamma$
: :				

INTEGRATION BY PARTS

$$\int u\frac{dv}{dx}dx = uv - \int v\frac{du}{dx}dx$$

TRAPEZOIDAL RULE

$$I = \int f(x)dx \approx \frac{h}{2}\{f(a)+2f(a+h)+2f(a+2h)+---+2f(a+(n-1)h)+f(b)\}$$

where $h=(b-a)/n$

SIMPSON'S RULE

$$I = \int_a^b f(x)dx = \frac{h}{3}\{f(a)+f(b)+4[f(a+h)+f(a+3h)+---+f(a+(n-1)h)] + 2[f(a+2h)+f(a+4h)+---+f(a+(n-2)h)]\}$$

where $h=(b-a)/n$ and n is even

HYPERBOLIC FUNCTIONS

$\cosh x = \frac{1}{2}(e^x + e^{-x})$;	$\sinh x = \frac{1}{2}(e^x - e^{-x})$;
$\tanh x = \frac{\sinh x}{\cosh x}$	$\cosh^2 x - \sinh^2 x = 1$;
$\cosh^2 x + \sinh^2 x = \cosh 2x$.	$2 \sinh x \cosh x = \sinh 2x$
$\cosh(-x) = \cosh x$	$\sinh(-x) = -\sinh x$

COMPLEX NUMBERS

$z = x + iy = re^{i\theta}$ $\quad (r \geq 0, -\pi \leq \theta < \pi)$

$e^{i\theta} = \cos\theta + i \sin\theta$; (Euler); $\quad (\cos\theta + i \sin\theta)^n = \cos n\theta + i \sin n\theta$ (De Moivre)

QUADRATIC EQUATIONS

$ax^2 + bx + c = 0$ has roots. $\quad x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ for real a, b, c.

The roots are complex if $b^2 < 4ac$ and real if $b^2 \geq 4ac$

FACTORIAL DEFINITIONS

$$n! = n(n-1)(n-2)\ldots\ldots 1 \qquad (0! = 1)$$

$${}^{n}C_{r} = \frac{n!}{(n-r)!\,r!}$$

BIONOMIAL SERIES

$$(x+y)^n = x^n + {}^{n}C_1\, x^{n-1}y + {}^{n}C_2\, x^{n-2}y^2 + \ldots. {}^{n}C_r\, x^{n-r}y^r + \ldots. + y^n$$

The coefficients in the binomial series, ${}^{n}C_{r}$, may be arranged as follows, with each line of the (Pascal) triangle corresponding to a different value of n:

n = 1							1		1						
n = 2						1		2		1					
n = 3					1		3		3		1				
n = 4				1		4		6		4		1			
n = 5			1		5		10		10		5		1		
n = 6		1		6		15		20		15		6		1	

The coefficients in non-end positions in the n^{th} line ($n \geq 3$) may be derived by adding the two coefficients in the $(n-1)^{th}$ line which are arranged diagonally to the left and to the right of the selected position in the n^{th} line.

DERIVATIVES AND INDEFINITE INTEGRALS OF ELEMENTARY FUNCTIONS

$f(x)$	$f'(x)=\frac{df(x)}{dx}$	$F(x)=\int f(x)dx$
x^n	nx^{n-1} $(n\neq 0)$	$x^{n+1}/(n+1)$, $(n\neq -1)$ $\ell n\, x$, $(n=-1)$
$\ell n\, x$	$1/x$	$x\,\ell n\, x - x$
e^{ax}	ae^{ax}	e^{ax}/a
$\sin x$	$\cos x$	$-\cos x$
$\cosh x$	$\sinh x$	$\sinh x$
$\sinh x$	$\cosh x$	$\cosh x$
$e^{f(x)}$	$f'(x)e^{f(x)}$	no general rule
$\sec^2 x$	$2\sec^2 x\ \tan x$	$\tan x$
$\frac{1}{(a^2-x^2)^{1/2}}$	$x(a^2-x^2)^{-3/2}$	$\sin^{-1}(x/a)$, $\lvert x\rvert<a$
$\tan x$	$\sec^2 x$	$-\ell n\lvert\cos x\rvert$

RULES FOR DIFFERENTIATION

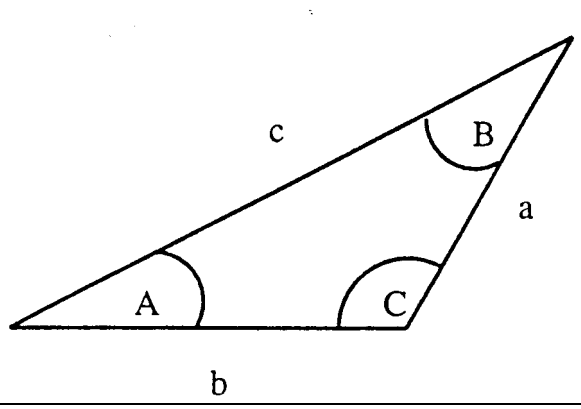
$$\frac{d}{dx}(fg)=f'g+fg'$$

$$\frac{d}{dx}(f/g)=(gf'-fg')/g^2$$

SCALOR, VECTOR PRODUCTS

a.**b** = |**a**| |**b**| cos C; *plane of*

a x **b** = |**a**| |**b**| sin C *n is unit vector, perpendicular to the the page and pointing towards the viewer.*



$$c^2 = a^2 + b^2 - 2ab\cos C;$$

$$\frac{a}{\sin A} = \frac{b}{\sin B} = \frac{c}{\sin C};$$

$$A + B + C = 180^\circ = \pi$$

MACLAURIN SERIES

$$f(x) = f(0) + \frac{f^{(1)}(0)}{1!}\cdot x + \frac{f^{(2)}(0)}{2!}\cdot x^2 + - - - + \frac{f^{(r)}(0)}{r!}\cdot x^r + - - -$$

TAYLOR SERIES

$$f(x) = f(a) + \frac{f^{(1)}(a)}{1!}\cdot (x-a) + \frac{f^{(2)}(a)}{2!}\cdot (x-a)^2 + \frac{f^{(r)}(a)}{r!}\cdot (x-a)^r + - - -$$

ARITHMETICAL PROGRESSION

$$S_n = a + (a+x) + (a+2x) + - - - + (a+(n-1)x) = \frac{n}{2}\left[2a + (n-1)x\right]$$

GEOMETRICAL PROGRESSION

$$S_n = a + ax + ax^2 + - - - + ax^{n-1} = \frac{a(1-x^n)}{1-x};\ \lim_{n\to\infty} S_n = \frac{a}{1-x},\quad \text{for } |x| < 1$$

TRIGOMETRICAL FORMULAE

Signs associated with values of the trigonometrical functions of angles in the various quadrants:

sin +	all +
tan +	cos +

all = sin, tan, cos

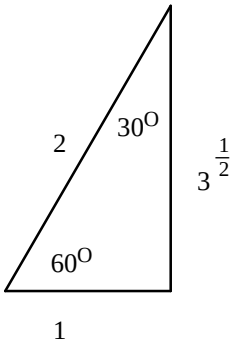
(π radians = 180º)

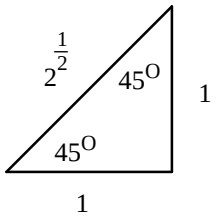
$\sin \pi = 0$; $\cos \pi = -1$; $\sin 0 = 0$; $\cos 0 = 1$;

$\sin \frac{\pi}{2} = 1$; $\cos \frac{\pi}{2} = 0$; $\sin \frac{\pi}{4} = \cos \frac{\pi}{4} = \frac{1}{\sqrt{2}}$;

$\sin \frac{\pi}{3} = \frac{\sqrt{3}}{2}$; $\cos \frac{\pi}{3} = \frac{1}{2}$; $\sin \frac{\pi}{6} = \frac{1}{2}$; $\cos \frac{\pi}{6} = \frac{\sqrt{3}}{2}$;

$\cos (-x) = \cos x$; $\sin (-x) = -\sin x$.





TRIGOMETRICAL FORMULAE continued....

$\cos^2 x + \sin^2 x = 1$;

$\cos (x \pm y) = \cos x \cos y \mp \sin x \sin y$;

$\sin (x \pm y) = \sin x \cos y \pm \cos x \sin y$;

$\tan x = \frac{\sin x}{\cos x}$; $\cot x = \frac{\cos x}{\sin x}$; $\sec x = \frac{1}{\cos x}$; $\operatorname{cosec} x = \frac{1}{\sin x}$

$\sin x \pm \sin y = 2 \sin \frac{1}{2}(x \pm y) \cos \frac{1}{2}(x \mp y)$;

$\cos x + \cos y = 2 \cos \frac{1}{2}(x + y) \cos \frac{1}{2}(x - y)$;

$\cos x - \cos y = 2 \sin \frac{1}{2}(x + y) \sin \frac{1}{2}(y - x)$;

$\cos 2x = \cos^2 x - \sin^2 x$; $\sin 2x = 2 \sin x \cos x$;

$\cos 3x = 4 \cos^3 x - 3 \cos x$; $\sin 3x = 3 \sin x - 4 \sin^3 x$;

$$\tan (x \pm y) = \frac{\tan x \pm \tan y}{1 \mp \tan x \tan y}$$

STUDENTS' t - DISTRIBUTION

Values exceeded in two-tailed test with probability P.

d.f	P = 0.1	0.05	0.02	0.01	0.002	0.001
1	6.314	12.706	31.821	63.657	318.31	636.62
2	2.920	4.303	6.965	9.925	22.327	31.598
3	2.353	3.182	4.541	5.841	10.214	12.924
4	2.132	2.776	3.747	4.604	7.173	8.610
5	2.015	2.571	3.365	4.032	5.893	6.869
6	1.943	2.447	3.143	3.707	5.208	5.959
7	1.895	2.365	2.998	3.499	4.785	5.408
8	1.860	2.306	2.896	3.355	4.501	5.041
9	1.833	2.262	2.821	3.250	4.297	4.781
10	1.812	2.228	2.764	3.169	4.144	4.587
11	1.796	2.201	2.718	3.106	4.025	4.437
12	1.782	2.179	2.681	3.055	3.930	4.318
13	1.771	2.160	2.650	3.012	3.852	4.221
14	1.761	2.145	2.624	2.977	3.787	4.140

15	1.753	2.131	2.602	2.947	3.733	4.073
16	1.746	2.120	2.583	2.921	3.686	4.015
17	1.740	2.110	2.567	2.898	3.646	3.965
18	1.734	2.101	2.552	2.878	3.610	3.922
19	1.729	2.093	2.539	2.861	3.579	3.883
20	1.725	2.086	2.528	2.845	3.552	3.850
21	1.721	2.080	2.518	2.831	3.527	3.819
22	1.717	2.074	2.508	2.819	3.505	3.792
23	1.714	2.069	2.500	2.807	3.485	3.767
24	1.711	2.064	2.492	2.797	3.467	3.745
25	1.708	2.060	2.485	2.787	3.450	3.725
26	1.706	2.056	2.479	2.779	3.435	3.707
27	1.703	2.052	2.473	2.771	3.421	3.690
28	1.701	2.048	2.467	2.763	3.408	3.674
29	1.699	2.045	2.462	2.756	3.396	3.659
30	1.697	2.042	2.457	2.750	3.385	3.646
40	1.684	2.021	2.423	2.704	3.307	3.551
60	1.671	2.000	2.390	2.660	3.232	3.460
120	1.658	1.980	2.358	2.617	3.160	3.373
∞	1.645	1.960	2.326	2.576	3.090	3.291

The last row of the table (∞) gives values of d, the unit (standard) normal deviate.

TOLERANCE INTERVALS

Level of Confidence	90%			95%		
% of items within tolerance interval / Sample size	90%	95%	99%	90%	95%	99%
3	5.85	6.92	8.97	8.38	9.92	12.86
4	4.17	4.94	6.44	5.37	6.37	8.30
5	3.49	4.15	5.42	4.28	5.08	6.63
6	3.13	3.72	4.87	3.71	4.41	5.78
7	2.90	3.45	4.52	3.31	4.01	5.25
8	2.74	3.26	4.28	3.14	3.73	4.89
9	2.63	3.13	4.10	2.97	3.53	4.63
10	2.54	3.02	3.96	2.84	3.38	4.43
12	2.40	2.86	3.76	2.66	3.16	4.15
14	2.31	2.76	3.62	2.53	3.01	3.96
16	2.25	2.68	3.51	2.44	2.90	3.81
18	2.19	2.61	3.43	2.37	2.82	3.70
20	2.15	2.56	3.37	2.31	2.75	3.62
30	2.03	2.41	3.17	2.14	2.55	3.35
40	1.96	2.33	3.07	2.05	2.45	3.21
50	1.92	2.28	3.00	2.00	2.38	3.13
Infinity	1.65	1.96	2.58	1.65	1.96	2.58

CRITICAL VALUES OF *F* FOR A ONE-TAILED TEST ($P = 0.05$)

(Source J C Miller and J N Miller (1993) Statistics for Analytical Chemistry, 3rd ed). Ellis Harwood

ν_2 / ν_1	1	2	3	4	5	6	7	8	9	10	12	15	20
1	161.4	199.5	215.7	224.6	230.2	234.0	236.8	238.9	240.5	241.9	243.9	245.9	248.0
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.41	19.43	19.45
3	10.13	9.552	9.277	9.117	9.013	8.941	8.887	8.845	8.812	8.786	8.745	8.703	8.660
4	7.709	6.944	6.591	6.388	6.256	6.163	6.094	6.041	5.999	5.964	5.912	5.858	5.803
5	6.608	5.786	5.409	5.192	5.050	4.950	4.876	4.818	4.772	4.735	4.678	4.619	4.558
6	5.987	5.143	4.757	4.534	4.387	4.284	4.207	4.147	4.099	4.060	4.000	3.938	3.874
7	5.591	4.737	4.347	4.120	3.972	3.866	3.787	3.726	3.677	3.637	3.575	3.511	3.445
8	5.318	4.459	4.066	3.838	3.687	3.581	3.500	3.438	3.388	3.347	3.284	3.218	3.150
9	5.117	4.256	3.863	3.633	3.482	3.374	3.293	3.230	3.179	3.137	3.073	3.006	2.936
10	4.965	4.103	3.708	3.478	3.326	3.217	3.135	3.072	3.020	2.978	2.913	2.845	2.774
11	4.844	3.982	3.587	3.357	3.204	3.095	3.012	2.948	2.896	2.854	2.788	2.719	2.646
12	4.747	3.885	3.490	3.259	3.106	2.996	2.913	2.849	2.796	2.753	2.687	2.617	2.544
13	4.667	3.806	3.411	3.179	3.025	2.915	2.832	2.767	2.714	2.671	2.604	2.533	2.459
14	4.600	3.739	3.344	3.112	2.958	2.848	2.764	2.699	2.646	2.602	2.534	2.463	2.388
15	4.543	3.682	3.287	3.056	2.901	2.790	2.707	2.641	2.588	2.544	2.475	2.403	2.328
16	4.494	3.634	3.239	3.007	2.852	2.741	2.657	2.591	2.538	2.494	2.425	2.352	2.276
17	4.451	3.592	3.197	2.965	2.810	2.699	3.614	2.548	2.494	2.450	2.381	2.308	2.230
18	4.414	3.555	3.160	2.928	2.773	2.661	2.577	2.510	2.456	2.412	2.342	2.269	2.191
19	4.381	3.522	3.127	2.895	2.740	2.628	2.544	2.477	2.423	2.378	2.308	2.234	2.155
20	4.351	3.493	3.098	2.866	2.711	2.599	2.514	2.447	2.393	2.348	2.278	2.203	2.124

ν_1 = number of degrees of freedom of the numerator and ν_2 = number of degrees of freedom of the denominator

NORMAL DISTRIBUTION (SINGLE-SIDED)

Proportion *(P)* of whole area lying to right of ordinate through $u = (\xi - \mu)/\sigma$

Deviate u	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
0.0	.5000	.4960	.4920	.4880	.4840	.4801	.4761	.4721	.4681	.4641
0.1	.4602	.4562	.4522	.4483	.4443	.4404	.4364	.4325	.4286	.4247
0.2	.4207	.4168	.4129	.4090	.4052	.4013	.3974	.3936	.3897	.3859
0.3	.3821	.3783	.3745	.3707	.3669	.3632	.3594	.3557	.3520	.3483
0.4	.3446	.3409	.3372	.3336	.3300	.3264	.3228	.3192	.3156	.3121
0.5	.3085	.3050	.3015	.2981	.2946	.2912	.2877	.2843	.2810	.2776
0.6	.2743	.2709	.2676	.2643	.2611	.2578	.2546	.2514	.2483	.2451
0.7	.2420	.2389	.2358	.2327	.2296	.2266	.2236	.2206	.2177	.2148
0.8	.2119	.2090	.2061	.2033	.2005	.1977	.1949	.1922	.1894	.1867
0.9	.1841	.1814	.1788	.1762	.1736	.1711	.1685	.1660	.1635	.1611
1.0	.1587	.1562	.1539	.1515	.1492	.1469	.1446	.1423	.1401	.1379
1.1	.1357	.1335	.1314	.1292	.1271	.1251	.1230	.1210	.1190	.1170
1.2	.1151	.1131	.1112	.1093	.1075	.1056	.1038	.1020	.1003	.0985
1.3	.0968	.0951	.0934	.0918	.0901	.0885	.0869	.0853	.0838	.0823
1.4	.0808	.0793	.0778	.0764	.0749	.0735	.0721	.0708	.0694	.0681

Deviate u	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
1.5	.0668	.0655	.0643	.0630	.0618	.0606	.0594	.0582	.0571	.0559
1.6	.0548	.0537	.0526	.0516	.0505	.0495	.0485	.0475	.0465	.0455
1.7	.0446	.0436	.0427	.0418	.0409	.0401	.0392	.0384	.0375	.0367
1.8	.0359	.0351	.0344	.0336	.0329	.0322	.0314	.0307	.0301	.0291
1.9	.0287	.0281	.0274	.0268	.0262	.0256	.0250	.0244	.0239	.0233
2.0	.0228	.0222	.0217	.0212	.0207	.0202	.0197	.0192	.0188	.0181
2.1	.0179	.0174	.0170	.0166	.0162	.0158	.0154	.0150	.0146	.0141
2.2	.0139	.0136	.0132	.0129	.0125	.0122	.0119	.0116	.0113	.0110
2.3	.0107	.0104	.0102		.00964		.00914		.00866	
2.4	.00820		.00776		.00734		.00695		.00657	
2.5	.00621		.00587		.00554		.00523		.00494	
2.6	.00466		.00440		.00415		.00391		.00368	
2.7	.00347		.00326		.00307		.00289		.00272	
2.8	.00256		.00240		.00226		.00212		.00199	
2.9	.00187		.00175		.00164		.00154		.00144	
3.0	0.00135									
3.5	0.000233									
Deviate u	**0.00**	**0.01**	**0.02**	**0.03**	**0.01**	**0.05**	**0.06**	**0.07**	**0.08**	**0.09**

PROBABILITY POINTS OF THE χ^2 DISTRIBUTION

∅	P														∅
	0.995	0.99	0.975	0.95	0.90	0.75	0.50	0.25	0.10	0.05	0.025	0.01	0.005	0.001	
1	--	--	--	--	0.16	0.102	.455	1.32	2.71	3.84	5.02	6.63	7.88	10.8	1
2	.010	.020	.051	.103	.211	.575	1.39	2.77	4.61	5.99	7.38	9.21	10.6	13.8	2
3	.072	.115	.216	.352	.584	1.21	2.37	4.11	6.25	7.81	9.35	11.3	12.8	16.3	3
4	.207	.297	.484	.711	1.06	1.92	3.36	5.39	7.78	9.49	11.1	13.3	14.9	18.5	4
5	.412	.554	.831	1.15	1.61	2.67	4.35	6.63	9.24	11.1	12.8	15.1	16.7	20.5	5
6	.676	.872	1.24	1.64	2.20	3.45	5.35	7.84	10.6	12.6	14.4	16.8	18.5	22.5	6
7	.989	1.24	1.69	2.17	2.83	4.25	6.35	9.04	12.0	14.1	16.0	18.5	20.3	24.3	7
8	1.34	1.65	2.18	2.73	3.49	5.07	7.34	10.2	13.4	15.5	17.5	20.1	22.0	26.1	8
9	1.73	2.09	2.70	3.33	4.17	5.90	8.34	11.4	14.7	16.9	19.0	21.7	23.6	27.9	9
10	2.16	2.56	3.25	3.94	4.87	6.74	9.34	12.5	16.0	18.3	20.5	23.2	25.2	29.6	10
11	2.60	3.05	3.82	4.57	5.58	7.58	10.3	13.7	17.3	19.7	21.9	24.7	26.8	31.3	11
12	3.07	3.57	4.40	5.23	6.30	8.44	11.3	14.8	18.5	21.0	23.3	26.2	28.3	32.9	12
13	3.57	4.11	5.01	5.89	7.04	9.30	12.3	16.0	19.8	22.4	24.7	27.7	29.8	34.5	13
14	4.07	4.66	5.63	6.57	7.79	10.2	13.3	17.1	21.1	23.7	26.1	29.1	31.3	36.1	14
15	4.60	5.23	6.26	7.26	8.55	11.0	14.3	18.2	22.3	25.0	27.5	30.6	32.8	37.7	15
16	5.14	5.81	6.91	7.96	9.31	11.9	15.3	19.4	23.5	26.3	28.8	32.0	34.3	39.3	16
17	5.70	6.41	7.56	8.67	10.1	12.8	16.3	20.5	24.8	27.6	30.2	33.4	35.7	40.8	17
18	6.26	7.01	8.23	9.39	10.9	13.7	17.3	21.6	26.0	28.9	31.5	34.8	37.2	42.3	18
19	6.84	7.63	8.91	10.1	11.7	14.6	18.3	22.7	27.2	30.1	32.9	36.2	38.6	43.8	19

FUNDAMENTAL CONSTANTS

Avogadro constant	L or N_A	6.022×10^{23} mol^{-1}
Bohr magneton	μ_B	9.274×10^{-24} J T^{-1}
Bohr radius	a_o	5.292×10^{-11} m
Boltzmann constant	k	1.381×10^{-23} J K^{-1}
charge of proton (charge of electron -e)	e	1.602×10^{-19} C
Faraday constant	$F = Le$	9.649×10^{4} C mol^{-1}
gas constant	$R = Lk$	8.314 J K^{-1} mol^{-1}
nuclear magneton	μ_N	5.051×10^{-27}J T^{-1}
permeability of a vacuum	μ_o	$4\pi \times 10^{-7}$ H m^{-1} or N A^{-2}
permittivity of a vacuum	$\varepsilon_0 = 1/\mu_o c^2$	8.854×10^{-12} F m^{1}
Planck constant	h	6.626×10^{-34} J s
(Planck constant)/2π	$\hbar$	1.054×10^{-34} J s
rest mass of electron	m or m_e	9.109×10^{-31} kg
rest mass of proton	m_p	1.673×10^{-27} kg
Rydberg constant	$R_\infty = me^4\mu_o^2c^3/8h^3$	1.097 373 x 10^7 m^{-1}
Speed of light in a vacuum	c	2.998×10^{8} m s^{-1}
Gravitational constant	G	6.673×10^{-11} N m^2 kg^{-2}
Atomic Mass Unit		1.66×10^{-27} kg

ln 10 - 2.3026; ln x = 2.3026 log x; log e = 0.4343; π = 3.14159;
R ln 10 = 19.144 J K^{-1} mol^{-1}; e = 2.7183;
(RT ln 10)/F = 59.16 mV at 298.2 K

SI UNITS

Quantity	Unit Name	Name Symbol
Length	metre	m
Mass	kilogram	kg
Time	second	s
Electric current	ampere	A
Thermodynamic temperature	kelvin	K
Amount of substance	mole	mol
Luminous intensity	candela	cd

Physical Quantity	Old Unit	New Unit	Basic Units	Conversion
Length	Angstrom (Å)	m		1 Å = 10^{-10} m
Energy	erg	J (joule)	kg m^2 s^{-2}	1 erg = 10^{-7} J
Force	dyne	N (newton)	kg m s^{-2}	1 dyne = 10^{-5} N
Pressure	atmosphere	Nm^{-2} + Pa (Pascal)		1 atmos = 1.013 × 10^5 Pa
	torr (mmHg)	Pa		1 torr = 133.3 Pa
		bar		1 bar = 10^5 Pa
Frequency	cycle/sec	Hz (hertz)	s^{-1}	1 c/s = 1 Hz
Force constant	dyne/cm	N m^{-1}	kg s^{-2}	
Mag. flux density	Gauss (G)	T (tesla)	kg s^{-2} A^{-1}	1 G = 10^{-4} T
Dipole moment	Debye (D)	C m		1 D = 3.334 ×10^{-30} C m
Radioactive exp.	Röntgen	C kg^{-1}		1 R = 2.58 × 10^{-4} C kg^{-1}

SPECIALLY NAMED MULTIPLES OF BASE 10

Fraction:	10^{12}	10^{9}	10^{6}	10^{3}	10^{-2}	10^{-3}	10^{-6}	10^{-9}	10^{-12}	10^{-15}	10^{-18}
SI prefix:	tera	giga	mega	kilo	centi	milli	micro	nano	pico	femto	atto
Symbol	T	G	M	k	c	m	μ	n	p	f	s

ATOMIC UNITS

Physical Quantity	Symbol	Value
Length	a_o	5.2918×10^{-11} m
Energy	E_h	4.3597×10^{-18} J
Dipole moment	ea_o	8.4784×10^{-30} C m