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Introduction

These Data pages contain 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).

Special thanks are due to Mrs May Price for her patience and skill in producing this Data Book Dr F N Manby for the point group flow chart.

C.B. Thomas

The Greek Alphabet

Alpha	A	α	Nu	N	ν
Beta	B	ß	Xi	Ξ	ξ
Gamma	Γ	γ	Omicron	O	o
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 12.8	Al 6.0	Si 8.2	P 10.5	S 10.4	Cl 13.0	Ar 15.8							
			K 4.3	Ca 6.1	Ga 6.0	Ge 7.9	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 -	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 6.8	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 5.4	Nd 5.5	Pm 5.6	Sm 5.6	Eu 5.7	Gd 6.1	Tb 5.8	Dy 5.9	Ho 6.0	Er 6.1	Tm 6.2	Yb 6.3	Lu 5.4				
Th 6.1	Pa 5.9	U 6.1	Np 6.2	Pa 6.1	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 -				

Single Bond Covalent Radii (in pm)

H 28	**C** 77	**N** 70	**O** 66	**F** 64
	Si 117	**P** 110	**S** 104	**Cl** 99
	Ge 122	**As** 121	**Se** 117	**Br** 114
	Sn 140	**Sb** 141	**Te** 137	**I** 133

Electron-Gain Energies

ΔU_0/kJ mol^{-1}

Periodic Table Arrangement

Li		**B**	**C**	**N**	**O**	**F**
-59.8		-7.5	-122.3	0	-141.1	-328.0
Na		**Al**	**Si**	**P**	**S**	**Cl**
-52.7		-44	-133.6	-72	-200.4	-348.8
K	**Cu**		**Ge**	**As**	**Se**	**Br**
-48.4	-118		-115	-77	-195.0	-324.6
Rb	**Ag**		**Sn**	**Sb**	**Te**	**I**
-46.9	-125.7		-120	-100	-190.2	-295.4
Cs	**Au**					
-45.5	-222.8					

Enthalpies of Formation of Gaseous Monatomic Cations

ΔH^{Θ}_{f} / kJ mol^{-1}

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

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 coordination numbers (c.n's) are given in the Notes below, and the values for species in **bold** give an appropriate idea of the sizes of these ions.

Oxidation State		(A) Non-transition Metals							
-3		**N**	**P**	**As**					
		150	**190**	**220**					
-2		O[c]	**S**	**Sc**	**Te**				
		140	**185**	**195**	**220**				
-1		F[d]	**Cl**	**Br**	**I**	**OH^-**	**SH^-**		
		133	**180**	**195**	**215**	**155**	**200**		
+1	Li[a]	Na	K	Rb	Cs	Tl	**NH_4^+**		
	74	102	138	149	170	150	**150**		
+2	Be[b]	Mg	Ca	Sr	Ba[f]	Zn	Cd	Pb	
	35	72	100	116	136	75	150	118	
+3		Al	Sc	Y	La				
		53	73	89	106				
+4			Ti	Zr					
			61	72					

(B) Transition Metals

		Ti	V	Cr	Mn	Fe	Co	Ni	Cu
+2	Low spin			73	67	61	65		
	High spin	86	79	82	82	77	74	70	73
+3	Low spin				58	55	53	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, 102 pm; c.n. 9, 110 pm
(f) c.n. 8, 142 pm; c.n. 12, 160 pm

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 2.06	**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	**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** 193 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** 135 1.22	**Nb** 143 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 1.08	**Hf** 155 1.23	**Ta** 145 1.33	**W** 135 1.40	**Re** 135 1.46	**Os** 130 1.52	**Ir** 135 1.55	**Pt** 135 1.44	**Au** 135 1.42	**Hg** 150 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 Salter (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	E⁰ /V	Oxidised/Reduced Species	E⁰ /V
Ag^+/Ag	+0.7991	K^+/K	-2.925
Ag^{2+}/Ag^+	+1.98		
$AgCl/Ag, Cl^-$	+0.222	La^{3+}/La	-2.52
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
$Br_2(l)/2Br^-$	+1.0652	$MnO_4^-, 8H^+/Mn^{2+}, 4H_2O$	+1.51
		$MnO_4^-, 4H^+/MnO_2, 2H_2O$	+1.695
Ca^{2+}/Ca	-2.87		
Cd^{2+}/Cd	-0.403	Na^+/Na	-2.714
$Cl_2/2Cl^-$	+1.3595	Ni^{2+}/Ni	-0.250
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

Reduction Potentials

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	$S_2O_8^{2-}/2SO_4^{2-}$	+2.01
Fe^{2+}/Fe	-0.440	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
$2H^+/H_2$	0.00	Ti^{2+}/Ti	-1.63
$H^+/H(g)$	-2.10	Ti^{3+}/Ti^{2+}	c -0.37
$½H_2/H^-$	-2.25	$(Ti^{IV}O)^{2+}, 2H^+/Ti^{3+}, H_2O$	+0.1
$H_3BO_3, 3H^+/B, 3H_2O$	-0.87	Tl^+/Tl	-0.3363
$H_2O_2, H^+/OH, H_2O$	+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
$2Hg^{2+}/Hg_2^{2+}$	+0.920	V^{3+}/V^{2+}	-0.255
		$VO^{2+}, 2H^+/V^{3+}, H_2O$	+0.361

$I_2/2I^-$	+0.5355		
$I_3^-/3I^-$	+0.536	Y^{3+}/Y	-2.37
In^{3+}/In	-0.342		
		Zn^{2+}/Zn	-0.763

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	(121.0)
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_6	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}.

Properties of Selected Organic Compounds

	Melting Point T_m/K	Boiling Point T_b/K	Density* ρ/kg m^{-3}	Enthalpy of formation *§ ΔH^o_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	g
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	$567^{\S\S}$	+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*
Methane	91	109	423^{+}	-75	g
Methanol	179	338	791	-239	*l*
Methoxymethane	135	250		-184	g
Methylbenzene	178	384	867	+12	*l*
2-methyl propane	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	g
1,3-Dimethylbenzene	225	412	864	+72	g
1,4-Dimethylbenzene	286	411	861	+75	g

* At 298 K;
§ A negative sign means evolution of heat;
** At 563 K.
+ At -111.5 K
§§ At 104K

Standard Enthalpies of Fusion and Vaporisation at the Transition Temperature

$\Delta_{trs}H^{\Theta}$ / (kJ mol^{-1})

	T_1/K	Fusion	T_b/K	Vaporisation
Elements				
Ag	1234	11.30	2436	250.6
At	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

Standard Enthalpies of Fusion and Vaporization at the Transition Temperature

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	18.08	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

$\Delta_{hyd}H^{\Theta}$ / (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

Entires 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

$\Delta_{hyd}H^{\Theta}$ / (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

Entires refer to $X^{++}(g) \rightarrow X\text{-}^{+}(aq$ 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)

Temperature, Pressure and Volume Relationship of Saturated Steam

Temperature		Pressure	Specific volume
T/K	**(ºC)**	**P/bar** abs**	**$V/m^3\ kg^{-1}$**
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		Density	Specific Heat Capacity	Specific Latent Heat of Vaporisation
T/K	(°C)	/kg m^{-3}	c_p /J kg^{-1} K^{-1}	*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.

Thermodynamic Data for Elements and Inorganic Compounds

(all values are for 298K)

	M/(g mol^{-1})	$\Delta_t H^\ominus$ / (kJ mol^{-1})	$\Delta_t G^\ominus$ / (JK mol^{-1})§	$S_{mt}^\ominus$ / (JK^{-1} mol^{-1})§	$C_{p.m}^\ominus$ / (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	-36.4	-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	
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
$CuO(s)$	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	32.27
$D_2O(l)$	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	
Fluorine					
$F_2(g)$	38.00	0	0	202.78	31.30
$F(g)$	19.00	+78.99	+61.91	158.75	22.74
$F^{-}(aq)$	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	-258.83	-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	+1.70	206.59	29.158
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	-742.1	87.40	103.85
Krypton					
Kr(g)	83.80	0	0	164.80	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
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	
$NO_4^-(aq)$	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	
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	66.75	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
KI(s)	166.01	-327.90	-324.89	106.32	52.93
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,α)(rhombic)	32.06	0	0	31.80	22.64
S(s,β)(monoclinic)	32.06	+0.33	+0.1	32.6	23.6
S^{2-}(aq)	32.06	+33.1	+85.8	-14.6	
SO_2(aq)	64.06	-296.83	-300.19	248.22	39.87
SO_3(aq)	80.06	-395.72	-371.06	256.76	50.67

Thermodynamic Data for Organic Compounds

(All Values are for 298K)

	M/(g mol^{-1})	$\Delta_t H^\ominus$ / (kJ mol^{-1})	$\Delta_t G^\ominus$ / (JK mol^{-1})§	$S_{mt}^\ominus$ / (JK^{-1} mol^{-1})§	$C_{p.m}^\ominus$ / (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) *cis*-2-butene	56.11	-6.99	+65.95	300.94	78.91
C_4H_8(g) *trans*-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	86.14	-198.7		204.3	
$C_6H_5CH_3$(l)	86.14	-50.5	+122.0	320.7	103.6
Alcohols and Phenols					

CH_3OH(l) methanol	32.04	-238.66	-166.27	126.8	81.6
C_2H_5OH(l) ethanol	46.07	-277.69	-174.78	160.7	111.46
C_6H_5OH(l) 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

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

	To→			
From ↓	**t oil eq**	**therms**	**MW h**	**GJ**
t coal	0.63	250	7.31	26.4
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 a coal burned in the UK is typically 25 - 30 GJ t^{-1}.

For electricity generated (MW h) from fossil fuels you need to take into account 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

Table of Energy Equivalents

Energy associated with	J	eV	calories	kW h	Hz	cm^{-1}	K	$J\ mol^{-1}$
l 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 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^{34}	1.841×10^{-40}	1	3.336×10^{-11}	4.800×10^{-11}	3.990×10^{-10}
1 cm^{-1}	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

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 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}

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

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 anum

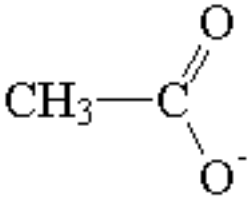
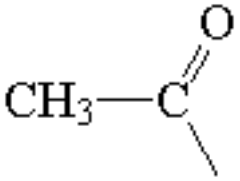
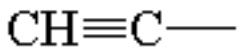
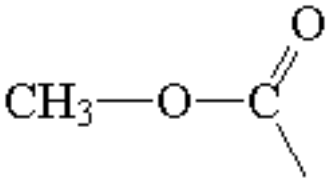
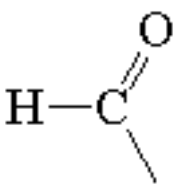
1. The Hadean, Archaean and Proterozoic together are commonly called Precambrian.
2. The Cambrian, Ordovician and Silurian are commonly classified as Lower Palaeozoic; and the Devonian, Carboniferous and Permian as Upper Palaeozoic.
3. Probable age of the Earth - 4560 Ma; oldest date rocks about 3800 Ma.

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

Typical Values of Hydrogen Atom Chemical Shifts

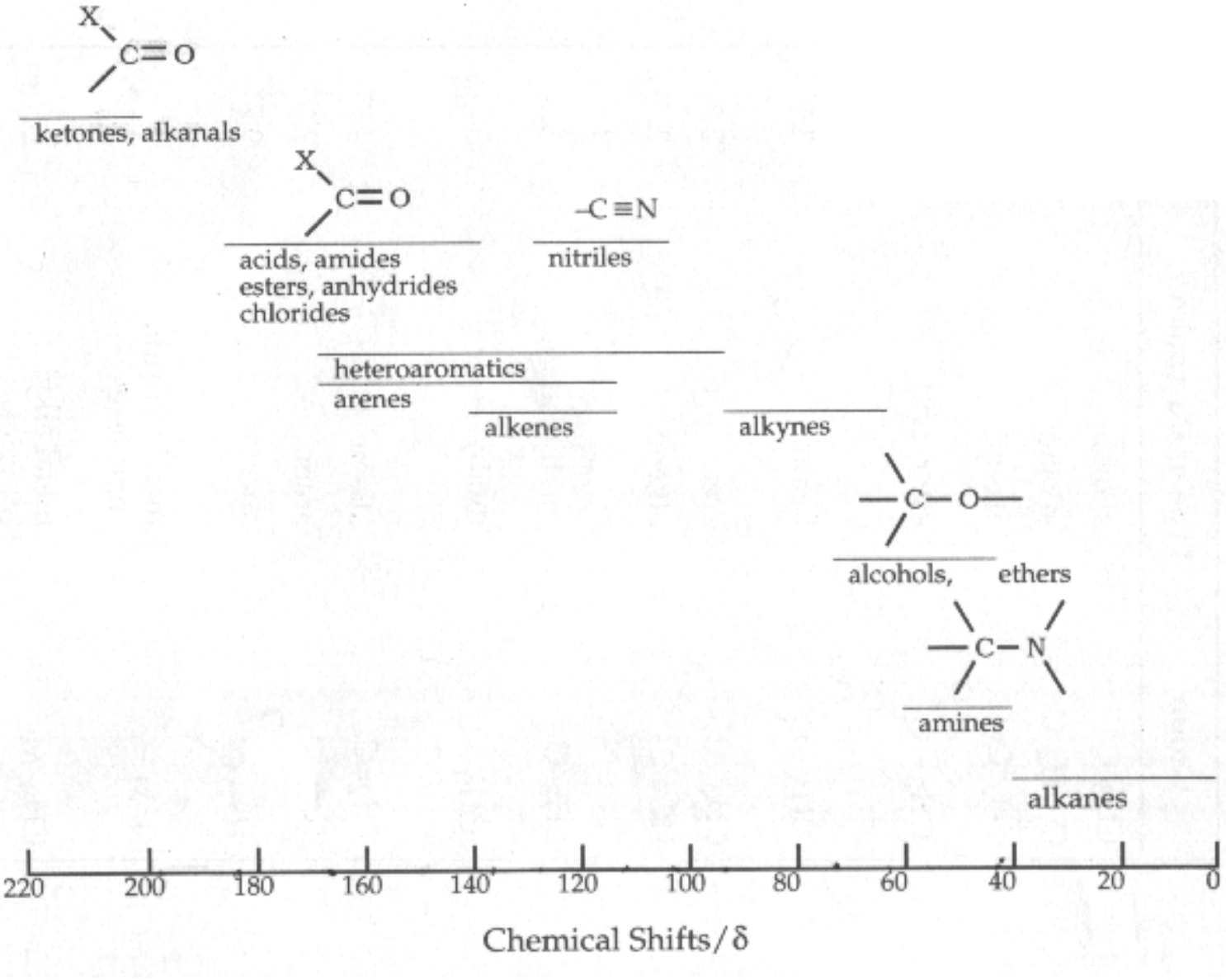
Group	Type of Compound	Chemical Shift/δ*
CH_3-Si	methylsilane	0.0
CH_3-C	alkane	0.9
C-CH_2-C	alkane	1.3
CH_3-C=C	alkene	1.6
	ester, acid	2.0
	ketone	2.2
CH_3-Ar	alkyl arene	2.3
CH_3-S	methyl thioether	2.1
	alkyne	2.0§
CH_3-N	amine	2.3
CH_3-O-	methyl ether	3.3
	methyl ester	3.7
CH_2=C	alkene	4.7§
H-C	arene	7.3§
	alkanal	9.7§

H-M	metal hydride complexes	$1 \rightarrow -40$
CH_3-M	metal alkyl complexes	$1 \rightarrow -1$

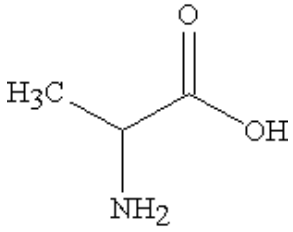
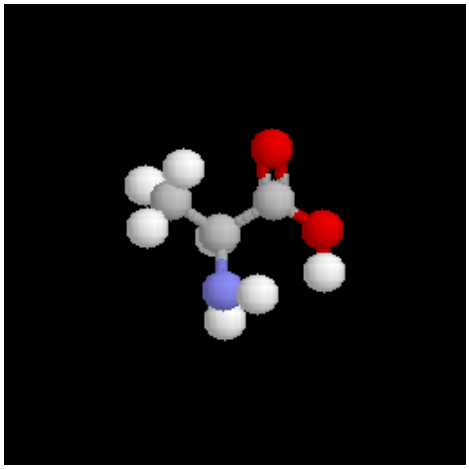
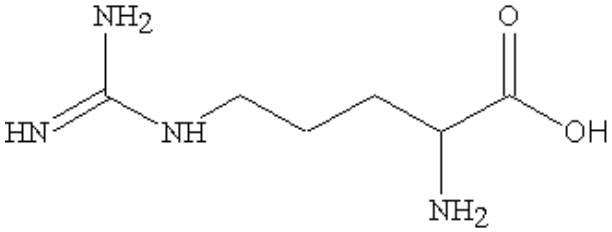
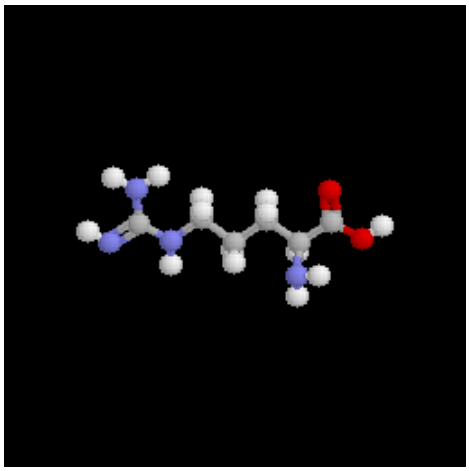
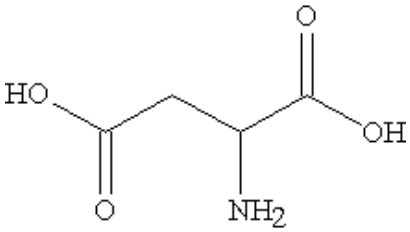
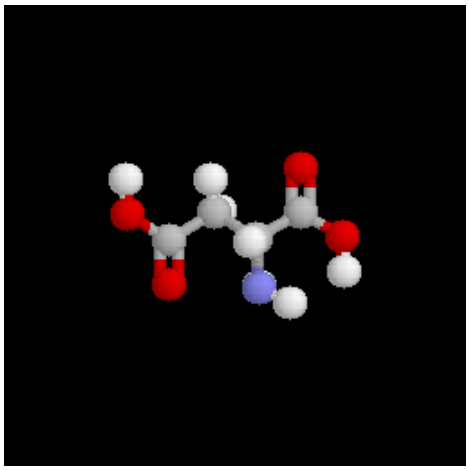
* Typically $\pm 0.1\delta$

§Substituent effects may cause a variation in the value listed.

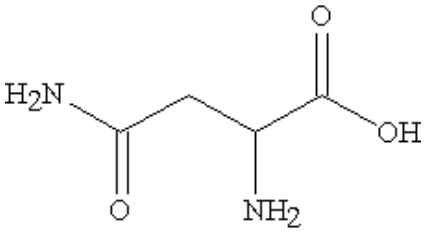
Ranges of ^{13}C NMR Chemical Shifts

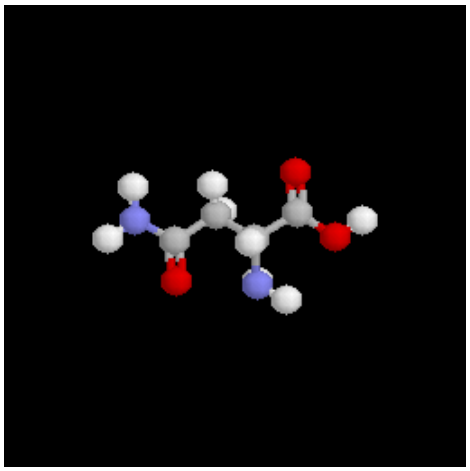


Amino Acids

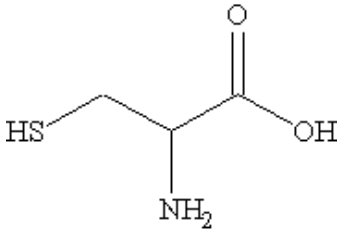
Name	Single letter code	Structure	3D Structure
alanine (Ala)	A		
arginine (Arg)	B		
aspartic acid (Asp)	D		

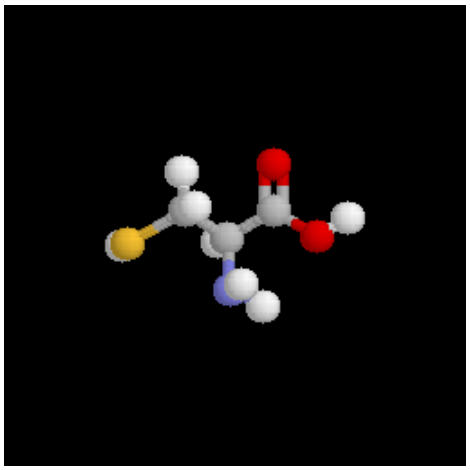
asparagine (Asn) N



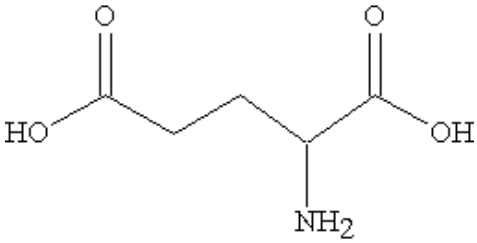


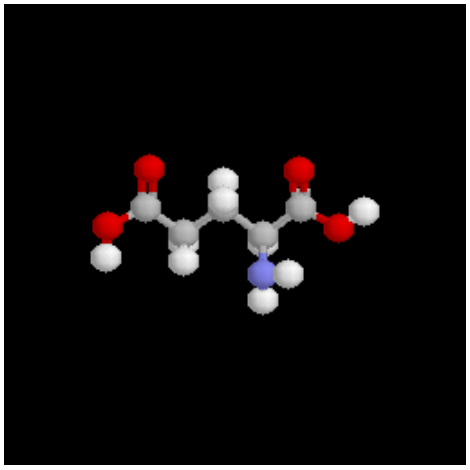
cysteine (Cys) C



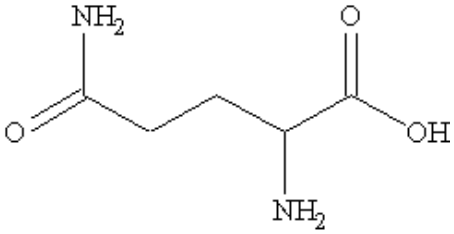


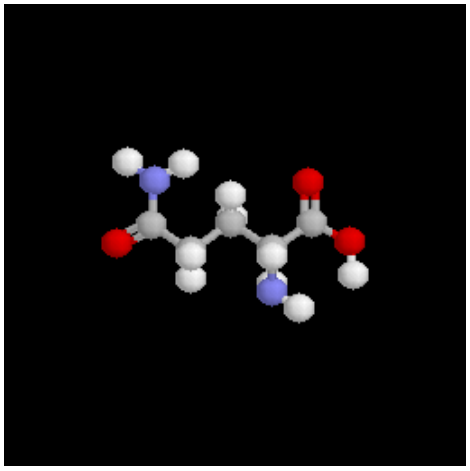
glutamic acid (Glu) E



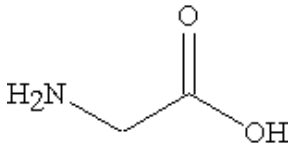


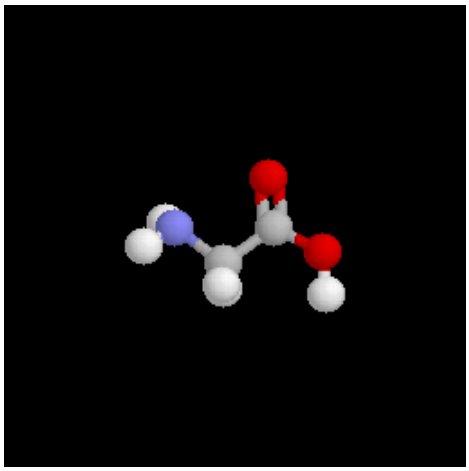
glutamine (Gln) Q



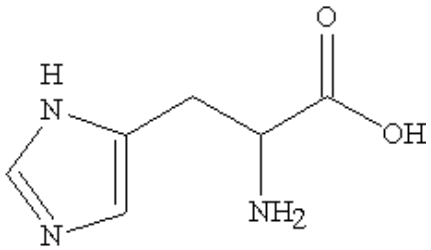


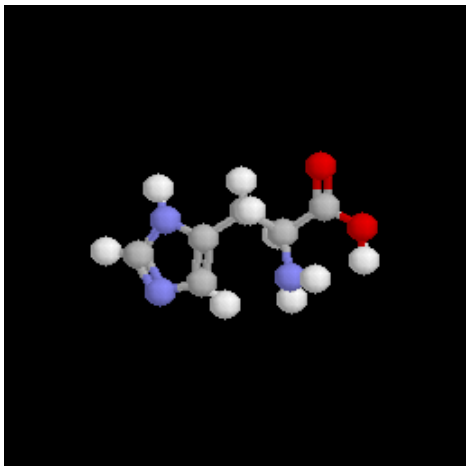
glycine (Gly) G



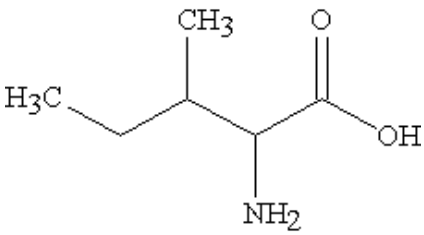


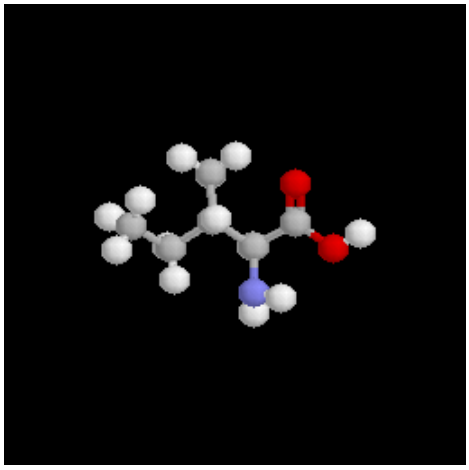
histidine (His) H



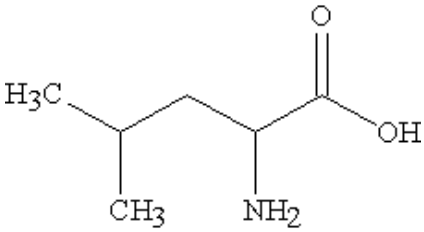


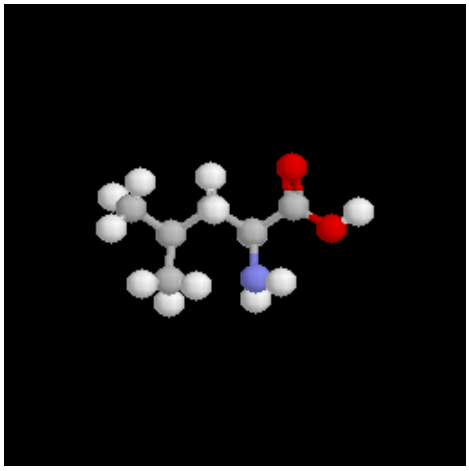
isoleucine (Ile) I



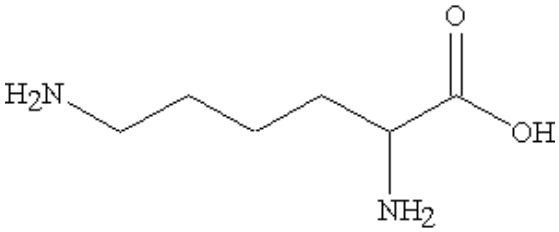


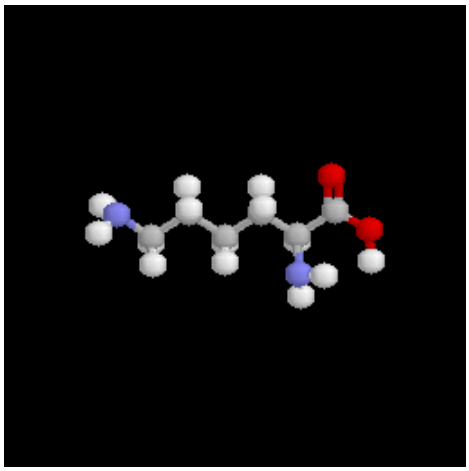
leucine (Leu) L



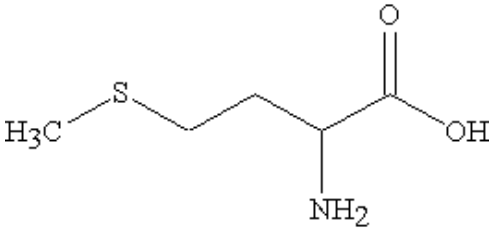


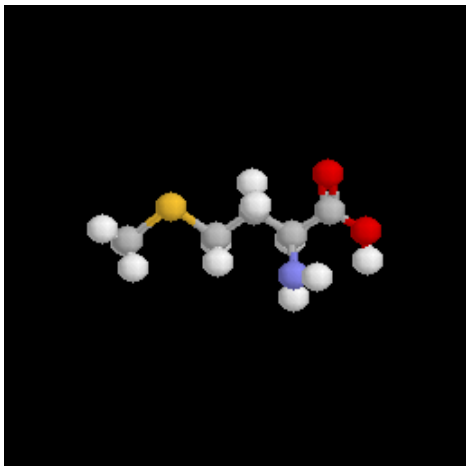
lysine (Lys) K



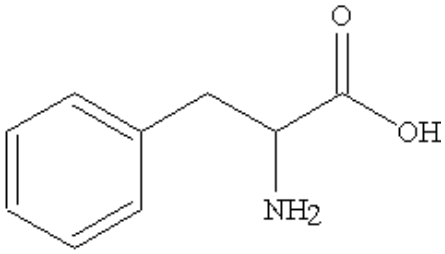


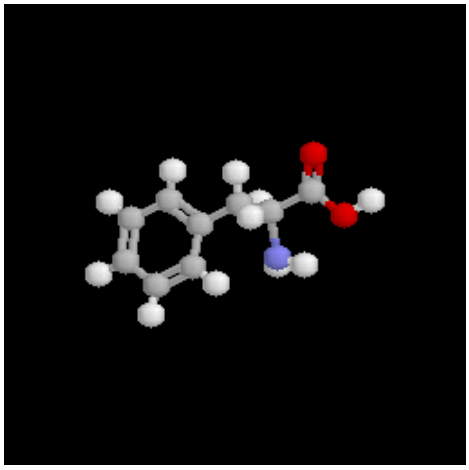
methionine (Met) M



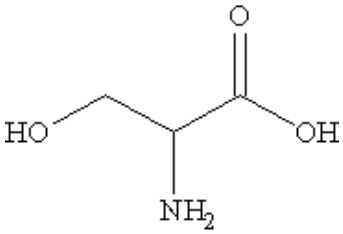


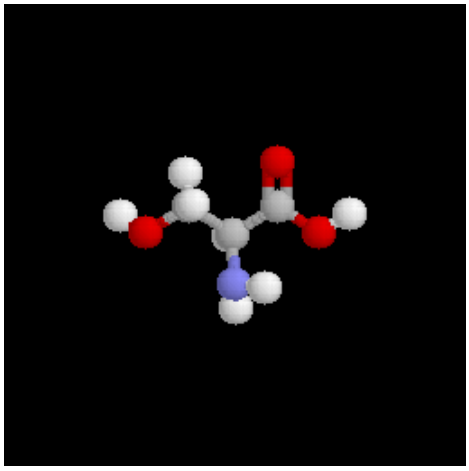
phenylalanine (Phe) F



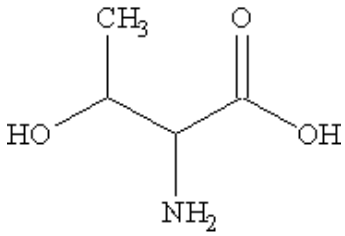


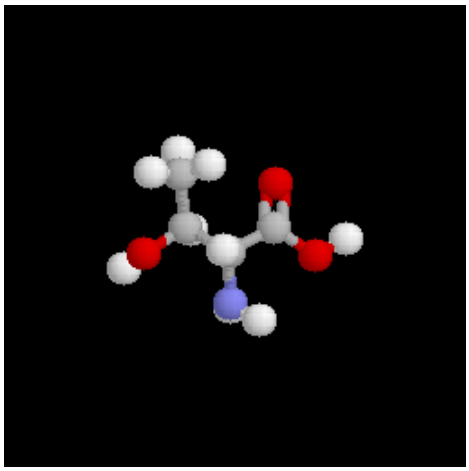
serine (Ser) S



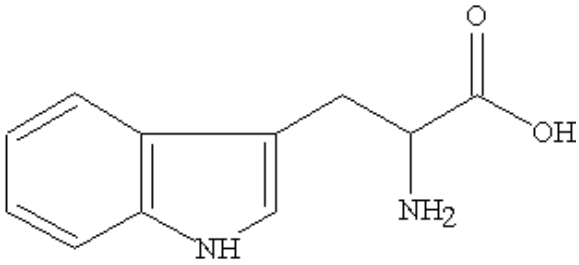


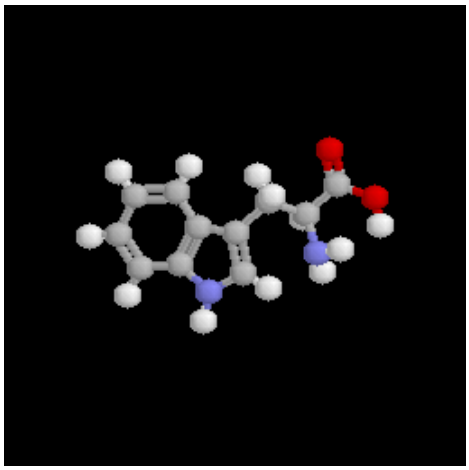
threonine (Thr) T



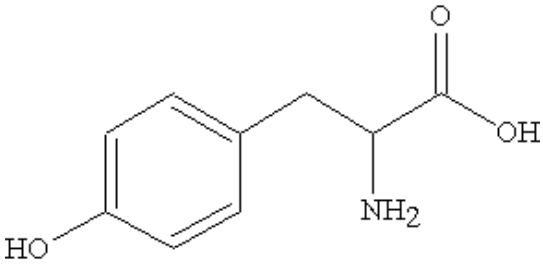


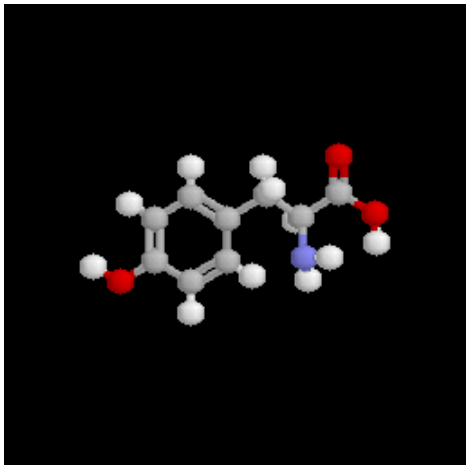
tryptophan (Trp) W



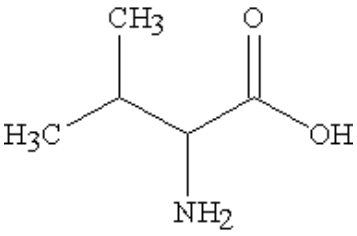


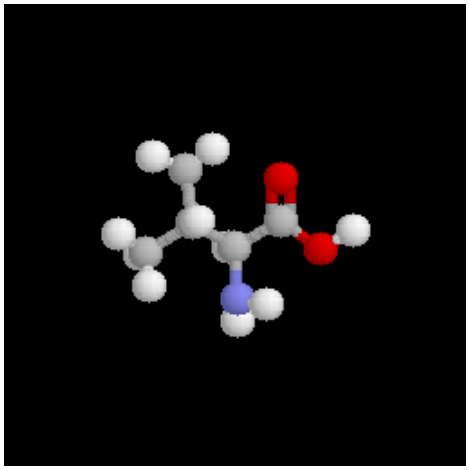
tyrosine (Tyr) Y



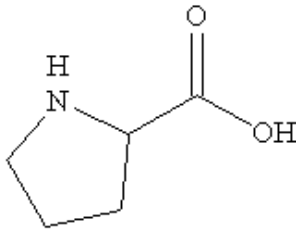


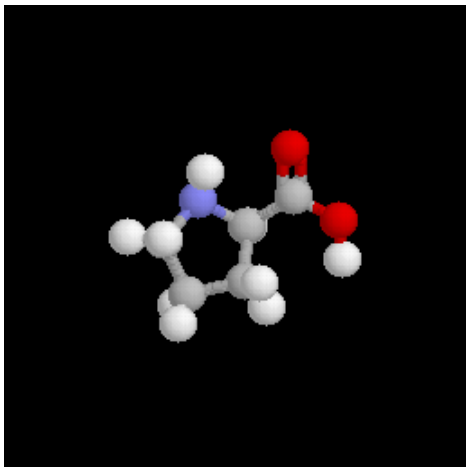
valine (Val) V





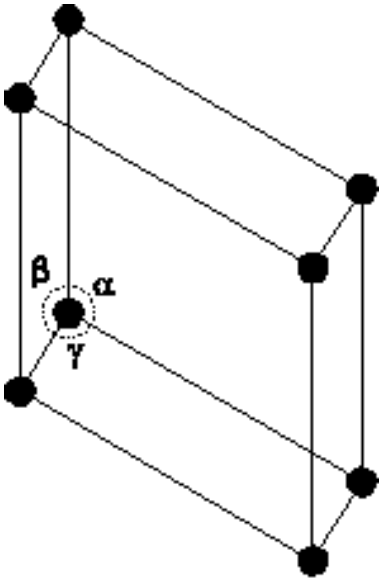
proline (Pro) P



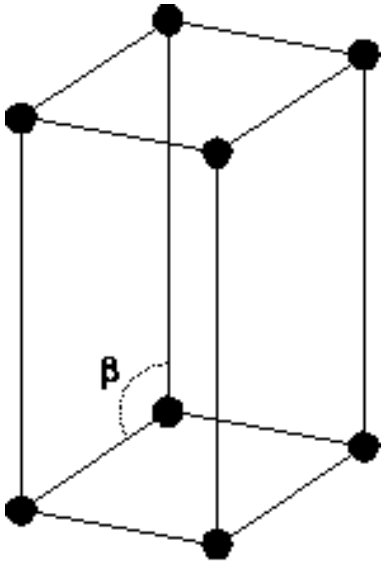


The Bravais Lattices

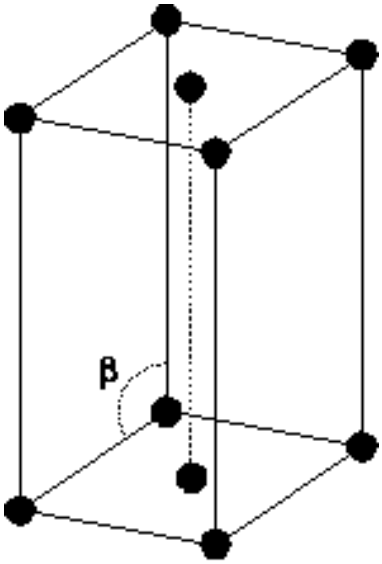
Instructions



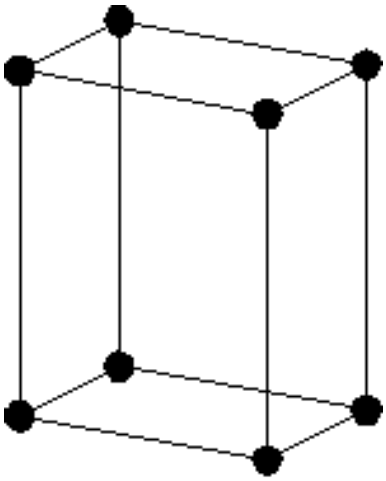
Triclinic (P)
$a \neq b \neq c$, $a \neq ß \neq \gamma \neq 90^o$



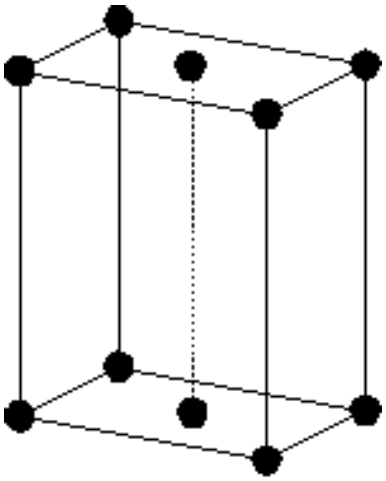
Monoclinic (P)
$a \neq b \neq c$, $\alpha = \gamma = 90^o$, $ß \neq 90^o$



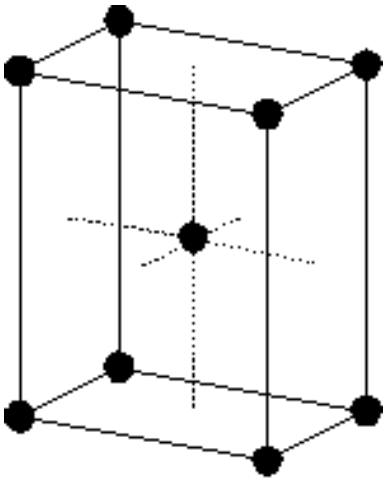
Monoclinic (C)
$a \neq b \neq c$, $\alpha = \gamma = 90^o$, $ß \neq 90^o$



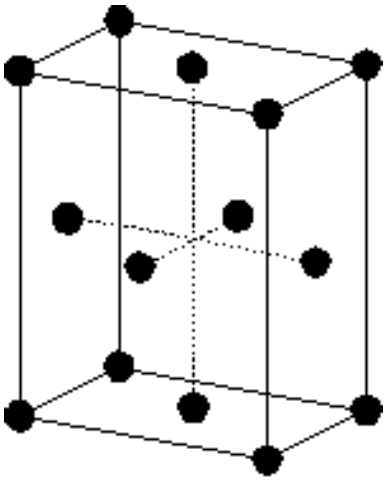
Orthorhombic (P)
$a \neq b \neq c$, $\alpha = ß = \gamma = 90^o$



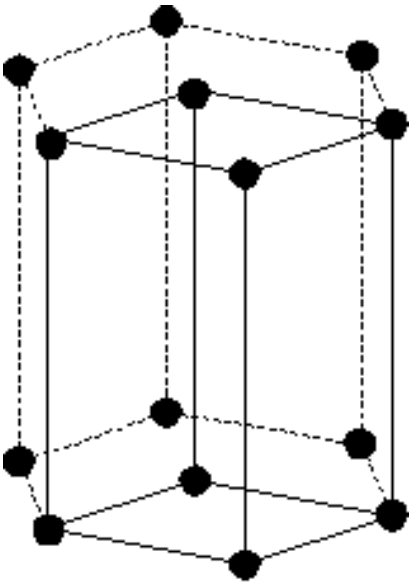
Orthorhombic (C)
$a \neq b \neq c$, $\alpha = ß = \gamma = 90^o$



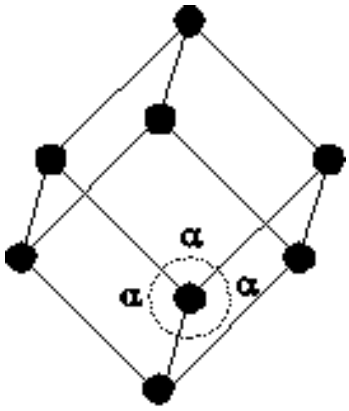
Orthorhombic (I)
$a \neq b \neq c$, $\alpha = ß = \gamma = 90^o$



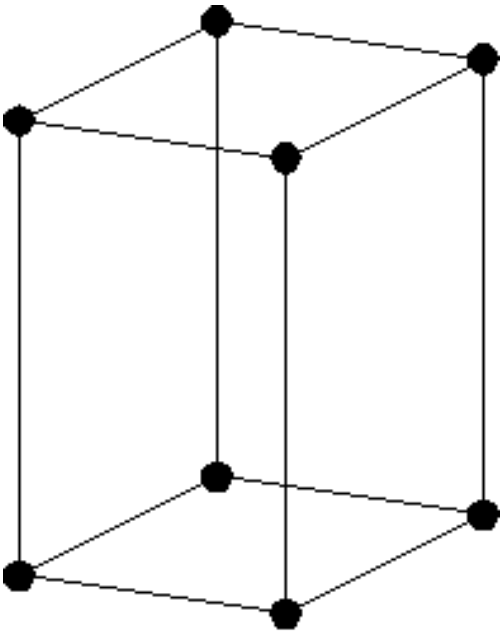
Orthorhombic (F)
$a \neq b \neq c$, $\alpha = ß = \gamma = 90^o$



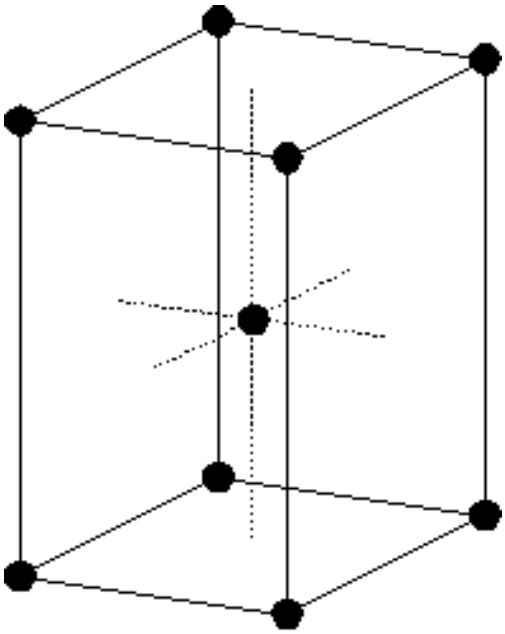
Hexagonal (P)
$a = b \neq c$, $\alpha = ß = 90^o$, $\gamma = 120^o$



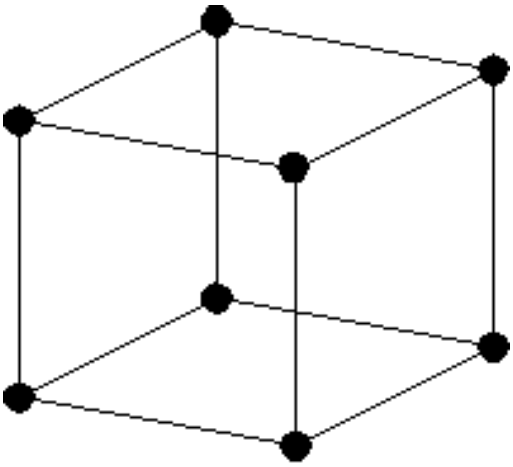
Rhombohedral (R)
$a = b = c$, $\alpha = ß = \gamma \neq 90^o$



Tetragonal (P)
$a = b \neq c$, $\alpha = ß = \gamma = 90^o$

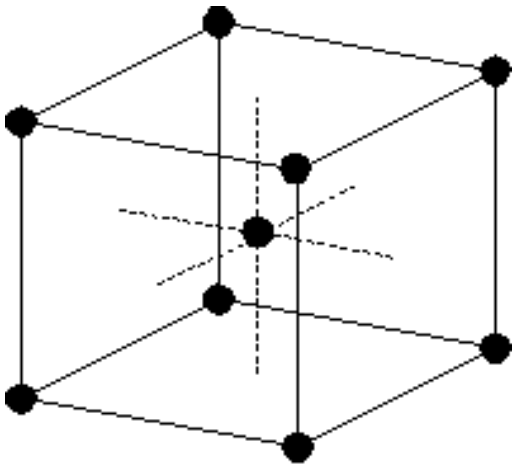


Tetragonal (I)
$a = b \neq c$, $\alpha = ß = \gamma = 90^o$

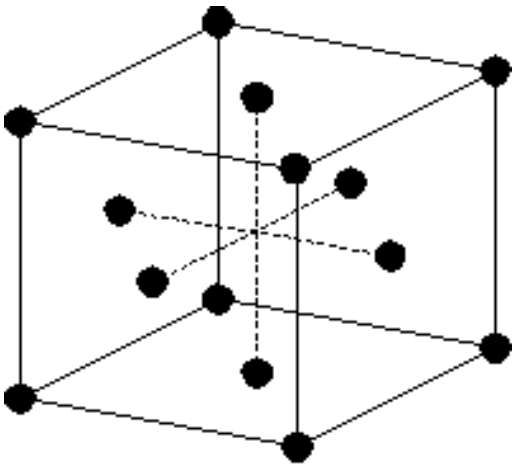


Cubic (P)
$a = b = c$, $\alpha = ß = \gamma = 90^o$

The Bravais Lattices



Cubic (I)
a = b = c, α = ß = γ = 90º



Cubic (F)
a = b = c, α = ß = γ = 90º

Common Abbreviations

Ar	any aryl group
BOC	-$CO_2{}^tBu$
CBZ (Z)	-CO_2Bn
MCPBA	meta-chloroperbenzoic acid (3-$ClC_6H_4CO_3H$
PCC	pyridinium chlorochromate ($C_5H_5N^+H\ ClCrO_3^-$)
R	any alkyl group
TBDMS(TBS)	-$SiMe_2{}^tBu$
TFA	trifluoroacetic acid, CF_3CO_2H
THF	tetrahydrofuran
THP	tetrahydropuran
TMS	-trimethylsilyl -$SiMe_3$

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**	
U	Phe	Ser	Tyr	Cys	**U**
	Phe	Ser	Tyr	Cys	**C**
	Leu	Ser	Stop	Stop	**A**
	Leu	Ser	Stop	Trp	**G**
C	Leu	Pro	His	Arg	**U**
	Leu	Pro	His	Arg	**C**
	Leu	Pro	Gln	Arg	**A**
	Leu	Pro	Gln	Arg	**G**
A	Ile	Thr	Asn	Ser	**U**
	Ile	Thr	Asn	Ser	**C**
	Ile	Thr	Lys	Arg	**A**
	Met	Thr	Lys	Arg	**G**
G	Val	Ala	Asp	Gly	**U**
	Val	Ala	Asp	Gly	**C**
	Val	Ala	Glu	Gly	**A**
	Val	Ala	Glu	Gly	**G**

Selected Hammett Substituent 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≡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

Infrared Absorption Frequencies for Some Inorganic Species

Species	ν/cm^{-1}
NO_3^-	1320 - 1420
SO_4^{2-}	1070 - 1130
ClO_4^-	1100 - 1150
PO_4^{3-}	1030 - 1100
CN^-	2240 - 2270
CrO_4^{2-}	840 - 900
MnO_4^-	770 - 810
BF_4^-	1040 - 1100
PF_6^-	800 - 880
NH_4^+	3200 - 3300
UO_2^{2+}	910 - 930
Terminal metal carbonyl, mono anion	2020 - 1750
Terminal metal carbonyl, neutral	2120 - 1820
μ_2-bridging metal carbonyl, neutral	1740 - 1880

Infrared Absorption Frequencies for Some Organic Functions

Vibration type	Molecule/Group		ν/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
	Arene (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
	Alkanomide		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 - 5150
		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; also peaks may show fine structure.

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)

NMR Properties and Relative Atomic Masses Of Stable Single Isotopes

Species	% Natural Abundance	Relative Isotopic Mass M/ g mol^{-1}	Receptivity (Relative to ^{13}C)	Nuclear Spin, I	Frequency/ MHz at 7.046 T	Electric Quadrupole Moment, $10^{28}Q/e\ m^2$
^{1}n	0.000	1.009	0.000000	1/2	205.607	0.000000
^{1}H	99.984	1.008	5680.000000	1/2	300.130	0.000000
^{2}H	0.016	2.014	0.008210	1	46.073	0.002800
^{3}H	0.000	3.016	0.000000	1/2	320.128	0.000000
^{3}He	0.000	3.016	0.003260	1/2	228.633	0.000000
^{6}Li	7.420	6.015	3.580000	1	44.167	0.000690
^{7}Li	92.580	7.016	1540.000000	3/2	116.640	-0.030000
^{9}Be	100.000	9.012	78.800003	3/2	42.174	0.051200
^{10}B	19.580	10.013	22.100000	3	32.246	0.074000
^{11}B	80.420	11.009	754.000000	3/2	96.258	0.035500
^{12}C	98.890	12.000	0.000000	0		0.000000
^{13}C	1.108	13.003	1.000000	1/2	75.468	0.000000
^{14}N	99.630	14.003	5.690000	1	21.687	0.016000
^{15}N	0.370	15.000	0.021900	1/2	30.424	0.000000
^{16}O	99.760	15.995	0.000000	0		0.000000
^{17}O	0.037	16.999	0.061100	5/2	40.686	-0.026000
^{18}O	0.204	17.999	0.000000	0		0.000000
^{19}F	100.000	18.998	4730.000000	1/2	282.404	0.000000
^{21}Ne	0.257	20.994	0.035900	3/2	23.692	0.090000
^{23}Na	100.000	22.990	525.000000	3/2	79.390	0.140000
^{25}Mg	10.130	24.986	1.540000	5/2	18.374	0.220000

^{27}Al	100.000	26.982	1170.000000	5/2	78.205	0.149000
^{28}Si	92.230	27.977	0.000000	0		0.000000
^{29}Si	4.670	28.976	2.090000	1/2	59.627	0.000000
^{30}Si	3.100	29.974	0.000000	2		0.000000
^{31}P	100.000	30.974	377.000000	1/2	121.496	0.000000
^{32}S	95.000	31.972	0.000000	0		0.000000
^{33}S	0.760	32.971	0.097300	3/2	23.038	-0.064000
^{34}S	4.22	33.968	0.000000	0		0.000000
^{35}Cl	75.530	34.969	20.200001	3/2	29.407	-0.078900
^{37}Cl	24.470	36.966	3.770000	3/2	24.479	-0.062100
^{39}K	93.080	38.964	2.690000	3/2	14.004	0.110000
^{41}K	6.880	40.962	0.032800	3/2	7.686	0.067000
^{43}Ca	0.145	42.959	0.052700	7/2	20.196	-0.050000
^{45}Sc	100.000	44.956	1710.000000	7/2	72.908	-0.220000
^{47}Ti	7.280	46.952	0.864000	5/2	16.924	0.290000
^{49}Ti	5.510	48.948	1.180000	7/2	16.920	0.240000
^{50}V	0.240	49.947	0.755000	6	29.923	0.210000
^{51}V	99.760	50.944	2160.000000	7/2	78.943	-0.052000
^{53}Cr	9.550	52.941	0.490000	3/2	16.963	0.030000
^{55}Mn	100.000	54.938	994.000000	5/2	74.267	0.550000
^{57}Fe	2.190	56.935	0.004190	1/2	9.718	0.000000
^{59}Co	100.000	58.933	1570.000000	7/2	71.212	0.400000
^{61}Ni	1.190	60.931	0.241000	3/2	26.820	0.160000
^{63}Cu	69.090	62.930	365.000000	3/2	79.618	-0.160000
^{65}Cu	30.910	64.928	201.000000	3/2	85.288	-0.150000

^{67}Zn	4.110	66.927	0.665000	5/2	18.779	0.150000
^{69}Ga	60.400	68.926	237.000000	3/2	72.034	0.178000
^{71}Ga	39.600	70.925	319.000000	3/2	91.531	0.112000
^{73}Ge	7.760	72.923	0.617000	9/2	10.469	-0.200000
^{75}As	100.000	74.922	143.000000	3/2	51.391	0.300000
^{77}Se	7.580	76.920	2.980000	1/2	57.241	0.000000
^{79}Br	50.540	78.918	226.000000	3/2	75.195	0.330000
^{81}Br	49.460	80.916	277.000000	3/2	81.056	0.280000
^{83}Kr	11.550	82.914	1.230000	9/2	11.542	0.150000
^{85}Rb	72.150	84.912	43.400002	5/2	28.965	0.270000
^{87}Rb	27.850	86.909	277.000000	3/2	98.206	0.130000
^{87}Sr	7.020	86.909	1.070000	9/2	13.008	0.200000
^{89}Y	100.000	88.906	0.668000	1/2	14.706	0.000000
^{91}Zr	11.230	90.905	6.040000	5/2	27.900	-0.210000
^{93}Nb	100.000	92.906	2740.000000	9/2	73.460	-0.200000
^{95}Mo	15.720	94.906	2.880000	5/2	19.559	0.120000
^{97}Mo	9.460	97.906	1.840000	5/2	19.971	1.100000
^{99}Tc	100.000	98.906	2130.000000	9/2	67.553	-0.190000
^{99}Ru	12.720	98.906	0.830000	5/2	13.848	0.076000
^{101}Ru	17.070	100.904	1.560000	5/2	15.520	0.440000
^{103}Rh	100.000	102.904	0.177000	1/2	9.559	0.000000
^{105}Pd	22.300	104.904	1.410000	5/2	13.734	0.800000
^{107}Ag	51.580	106.905	0.195000	1/2	12.149	0.000000
^{109}Ag	48.180	108.904	0.276000	1/2	13.968	0.000000
^{111}Cd	12.750	110.904	6.930000	1/2	63.631	0.000000

^{113}Cd	12.260	112.904	7.600000	1/2	66.563	0.000000
^{113}In	4.280	112.904	83.800003	9/2	65.626	1.140000
^{115}In	95.720	114.904	1890.000000	9/2	65.767	1.160000
^{117}Sn	7.610	116.903	19.500000	1/2	106.942	0.000000
^{119}Sn	8.580	118.903	25.200001	1/2	111.921	0.000000
^{121}Sb	57.250	120.903	520.000000	5/2	71.824	-0.500000
^{123}Sb	42.750	122.904	111.000000	7/2	38.894	-0.700000
^{123}Te	0.870	122.904	0.890000	1/2	78.544	0.000000
^{125}Te	6.990	124.904	12.500000	1/2	94.691	0.000000
^{127}I	100.000	126.904	530.000000	5/2	60.053	-0.690000
^{129}Xe	2.440	128.904	31.799999	1/2	83.010	0.000000
^{131}Xe	21.180	130.905	3.310000	3/2	24.611	-0.120000
^{133}Cs	100.000	132.905	269.000000	7/2	39.865	-0.003000
^{135}Ba	6.590	134.905	83.000000	3/2	29.815	0.250000
^{137}Ba	11.320	136.905	4.410000	3/2	33.353	0.200000
^{138}La	0.089	137.905	0.430000	5	39.599	2.700000
^{139}La	99.911	138.908	336.000000	7/2	42.396	0.210000
^{141}Pr	100.000	140.900	1650.000000	5/2	87.911	-0.059000
^{143}Nd	12.700	142.909	2.340000	7/2	16.318	-0.480000
^{145}Nd	8.300	144.912	0.370000	7/2	10.039	-0.250000
^{147}Sm	14.950	146.914	1.260000	7/2	12.389	-0.208000
^{149}Sm	13.830	148.916	0.590000	7/2	9.871	0.060000
^{151}Eu	47.820	150.919	483.000000	5/2	74.435	1.160000
^{153}Eu	52.180	152.920	45.299999	5/2	32.867	2.900000
^{155}Gd	14.730	154.922	0.233000	3/2	11.462	1.600000

^{157}Gd	15.680	156.923	0.484000	3/2	14.328	2.000000
^{159}Tb	100.000	158.925	331.000000	3/2	68.063	1.300000
^{161}Dy	18.880	160.926	0.447000	5/2	9.886	1.400000
^{163}Dy	24.970	162.928	1.580000	5/2	13.755	1.600000
^{165}Ho	100.000	164.930	1020.000000	7/2	61.566	2.820000
^{167}Er	22.940	166.932	0.659000	7/2	8.674	2.830000
^{169}Tm	100.000	168.934	3.210000	1/2	24.824	0.000000
^{171}Yb	14.310	170.936	4.440000	1/2	52.862	0.000000
^{173}Yb	16.130	172.939	1.220000	5/2	14.562	2.800000
^{175}Lu	97.410	174.940	172.000000	7/2	34.236	5.680000
^{176}Lu	2.590	175.942	5.470000	7	23.794	8.000000
^{177}Hf	18.500	176.943	0.670000	7/2	9.364	3.000000
^{179}Hf	13.750	178.946	0.169000	9/2	5.609	3.000000
^{181}Ta	99.988	180.948	204.000000	7/2	35.986	3.000000
^{183}W	14.400	182.950	0.058900	1/2	12.503	0.000000
^{185}Re	37.070	184.953	280.000000	5/2	67.604	2.800000
^{187}Re	62.930	186.956	490.000000	5/2	68.286	2.600000
^{187}Os	1.640	186.956	0.001140	1/2	6.849	0.000000
^{189}Os	16.100	188.958	2.130000	3/2	23.305	0.800000
^{191}Ir	37.300	190.961	0.023000	3/2	5.156	1.500000
^{193}Ir	62.700	192.963	0.116000	3/2	5.615	1.500000
^{195}Pt	33.800	194.965	19.100000	1/2	64.414	0.000000
^{197}Au	100.000	196.966	0.143000	3/2	5.189	0.590000
^{199}Hg	16.840	198.966	5.420000	1/2	53.756	0.000000
^{201}Hg	13.220	200.970	1.080000	3/2	19.845	0.500000

^{203}Tl	29.500	202.972	289.000000	1/2	171.746	0.000000
^{205}Tl	70.500	204.974	769.000000	1/2	173.433	0.000000
^{207}Pb	22.600	206.976	11.800000	1/2	62.601	0.000000
^{209}Bi	100.000	208.980	777.000000	9/2	48.228	-0.400000
^{235}U	0.720	235.044	0.004950	7/2	5.372	4.100000
electron		0.000	3730000.000000	1/2	197000.000	0.000000

Table A: Order of Precedence for Groups

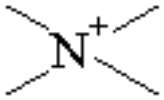
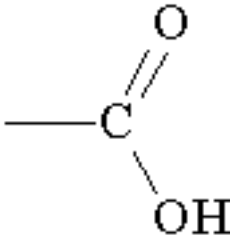
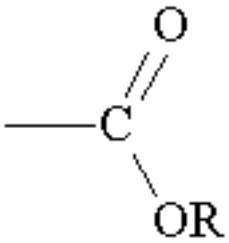
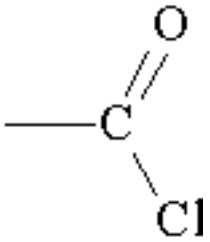
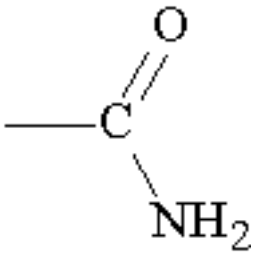
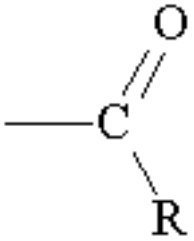
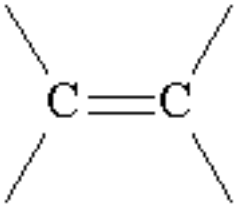
	-ammonium	
	-oic acid* -carboxylic acid†	carboxy-
	alkyl-oate* alkylcarboxylate†	alkoxycarbonyl-
$-SO_3H$	-sulfonic acid	sulfo-
	-oyl chloride* -carbonyl chloride†	chlorocarbonyl-
	-amide* -carboamide†	carbamoyl-
-CHO	-al* -carbaldehyde†	oxo-* methanoyl-†
	-one	oxo-* alkanoyl-†
-C≡N	-onitrile* -carbonitrile†	cyano-

Table A Order of Precedence for Groups

-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 a substituent on, e.g., a ring

Table B: Substituents Named Only As Prefixes

Group	Prefix
-OR	alkyloxy-
-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 (e.g., methyl, phenyl, cyclohexyl, indol-3-yl) unless they are chosen as the principal part of the structure.

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 293 K, $\gamma = c_p/c_v$**	**Viscosity at 293 K, $10^6\eta$/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 sulphide	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

Sulphur 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} l/J kg^{-1}	Specific heat capacity c_p/J kg^{-1} K^{-1}	Cubic Expansivity $10^{-5}\gamma/K^{-1}$	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 disulphide	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

Selected Physical Properties of Some Solid Materials

	Melting Point T_m/ K	**Density $10^{-3}\rho$/ kg m^{-3}**	**Specific enthalpy of fusion 10^{-4}1/J kg^{-1}**	**Specific heat capacity 10^{-2} c_p/J kg^{-1} K^{-1}**	**Linear expansivity 10^6 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 (70 Cu/30 Zn)	1300	8.5		3.7	18	110
Brick (building)		2.3			9	0.6
Brick (firebrick)		2.1			5	0.8
Bronze (90 Cu/10 Sn)	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 (60 Cu/40 Ni)	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/36 Ni)	1800	8.0		5	1	
Iron	1810	7.9	27	1.1	12	80
Iron (cast)	~1450	~7.5	~12		11	75
Lead	600	11.3	3	1.3	30	35
Manganin (83 Cu/15 Mn/3 Ni)		8.5	40	4	18	22
Monel (70 Ni/30 Cu)	1600	8.8			14	21

Selected Physical Properties of Some Solid Materials

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	
Sulphur	386	2.1		7	64	0.3
Sodium	370	0.97	11	12	71	134
Stainless Steel (18 Cr/8 Ni)	~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

Approximate pK_A Values of Selected Organic Compounds

Acid	Base	pK_a
RCO_2H	RCO_2^-	4 - 5
$PhOH$	PhO^-	10
$RCOCH_2CO_2R$	$RCOC^-HCO2R$	11
RCH_2OH	RCH_2O^-	16
$RCOCH_2R$	$RCOC^-HR$	19
$RC{\equiv}CH$	$RC{\equiv}C^-$	25
$R_2C{=}CH_2$	$R_2C{=}C^-H$	44
RCH_3	RC^-H_2	50

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 298K)

Ag^{+}	+	$2NH_3$	=	$[Ag(NH_3)_2]^{+}$	7.2
Co^{3+}	+	$6NH_3$	=	$[Co(NH_3)_6]^{3+}$	33.7
Cu^{2+}	+	$4NH_3$	=	$[Cu(NH_3)_4]^{2+}$	13.1
Zn^{2+}	+	$4NH_3$	=	$[Zn(NH_3)_4]^{2+}$	9.6
Ag^{+}	+	$2CN^{-}$	=	$[Ag(CN)_2]^{-}$	21.0
Fe^{3+}	+	$6CN^{-}$	=	$[Fe(CN)_6]^{3-}$	*ca* 31
Cu^{+}	+	$4CN^{-}$	=	$[Cu(CN)_4]^{3-}$	27.3
Zn^{2+}	+	$4CN^{-}$	=	$[Zn(CN)_4]^{2-}$	16.7
Ag^{+}	+	$EDTA^{4-}$	=	$[Ag(EDTA)]^{3-}$	7.3
Ca^{2+}	+	$EDTA^{4-}$	=	$[Ca(EDTA)]^{2-}$	10.7
Co^{3+}	+	$EDTA^{4-}$	=	$[Co(EDTA)]^{-}$	36
Cu^{2+}	+	$EDTA^{4-}$	=	$[Cu(EDTA)]^{2-}$	18.8
Fe^{3+}	+	$EDTA^{4-}$	=	$[Fe(EDTA)]^{-}$	25.1
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

Stokes' Law Of Viscosity

$v = 2gr^2(\rho - \rho_0)/(9\eta)$

where

v is the terminal velocity of fall of a spherical particle in a viscous medium

r is the radius of the particle

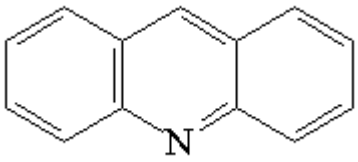
ρ is the density of the particle

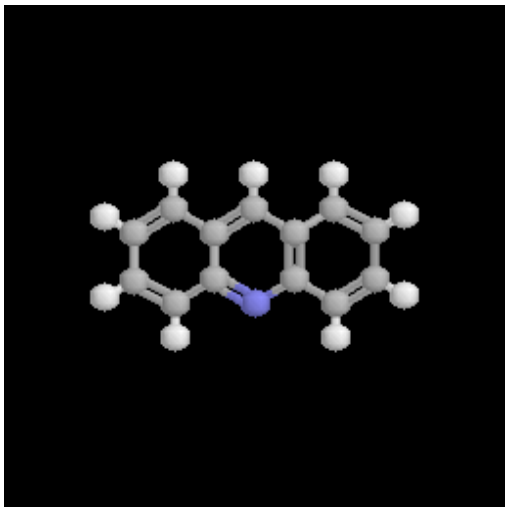
ρ_0 is the density of the medium

η is the coefficient of the medium

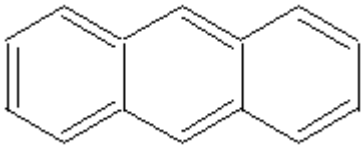
Structures of Selected Cyclic Organic Compounds

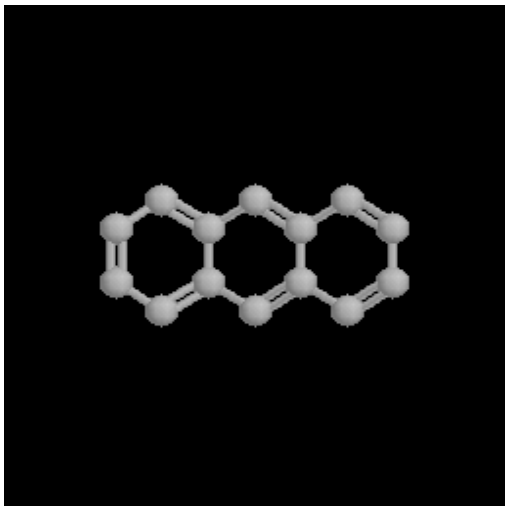
Acridine



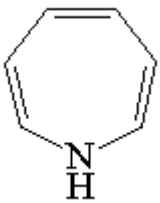


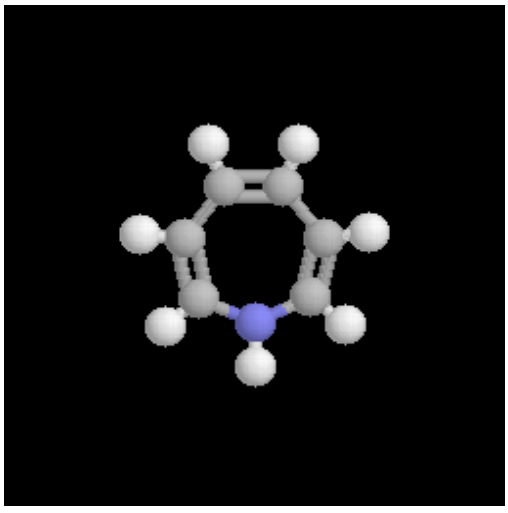
Anthracene



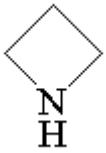


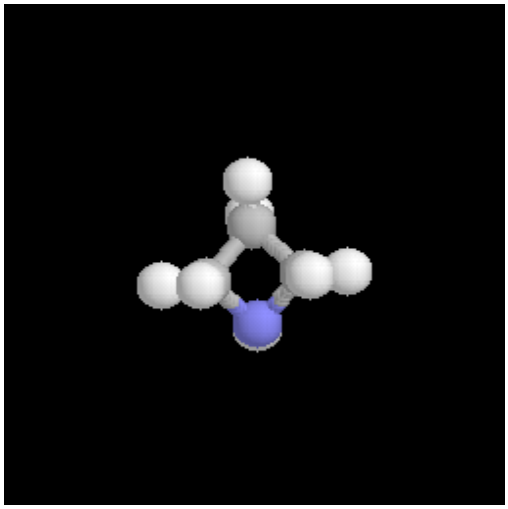
Azepine



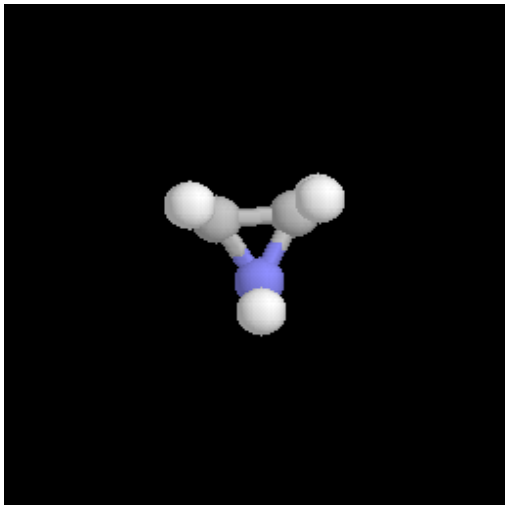


Azetidine

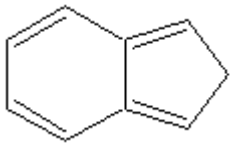


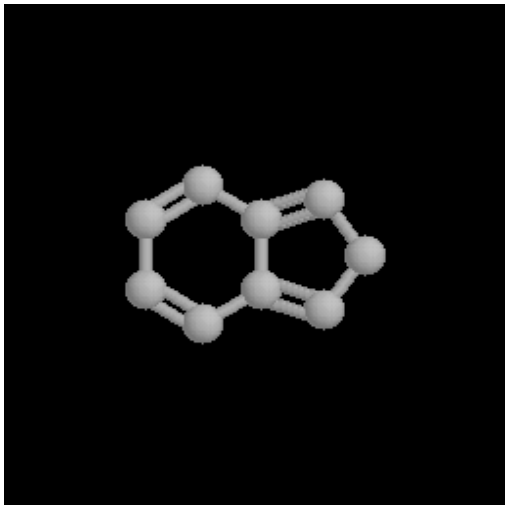


Aziridine

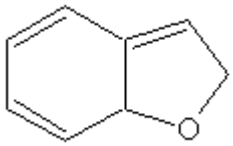


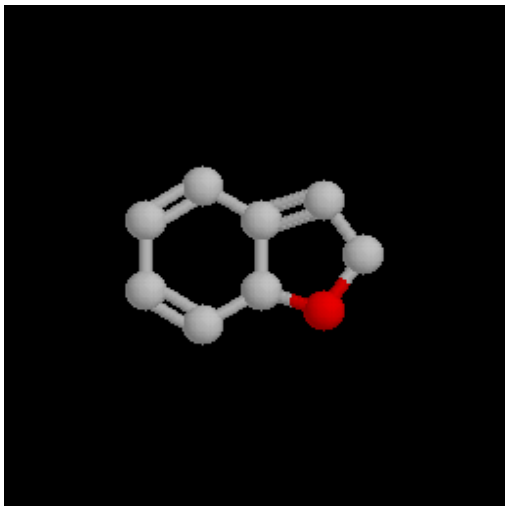
Azulene



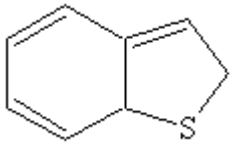


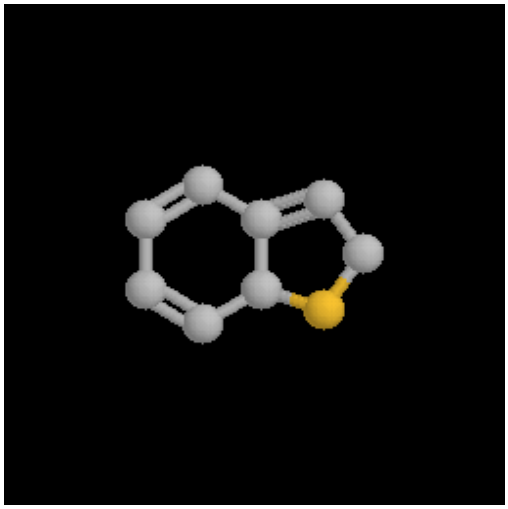
Benzoturan



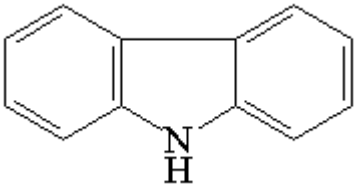


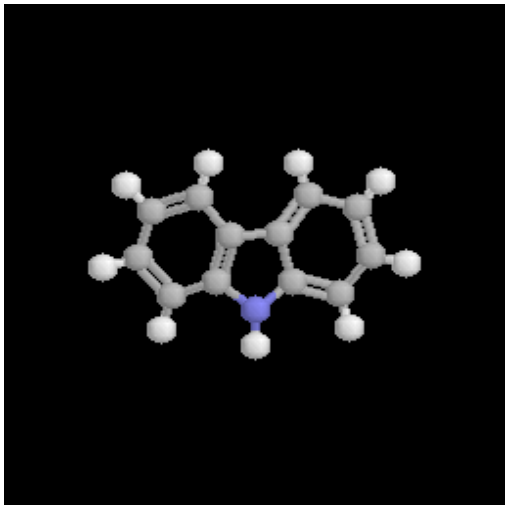
Benzothiophen



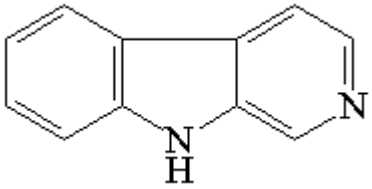


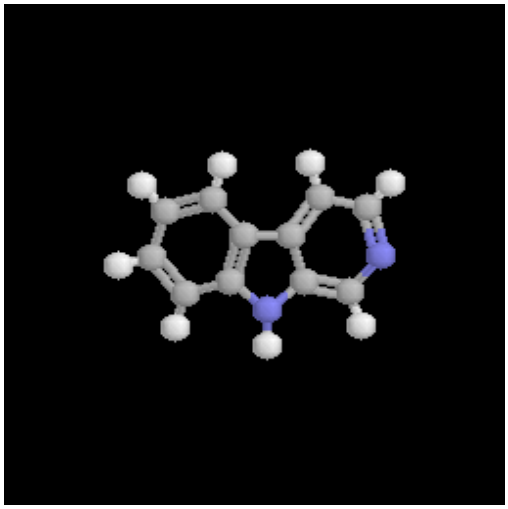
Carbazole



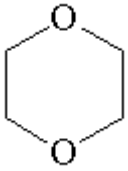


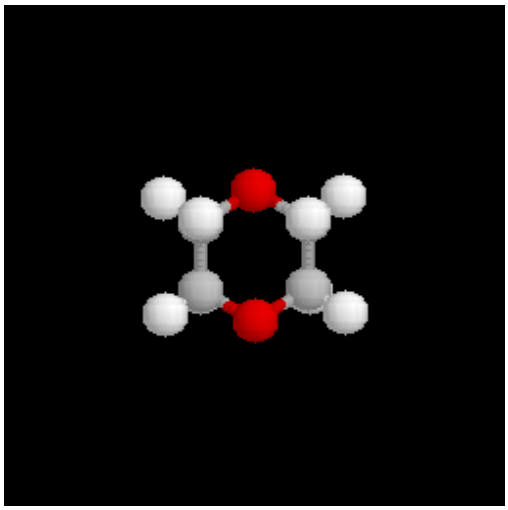
ß-Carboline



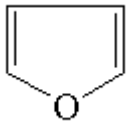


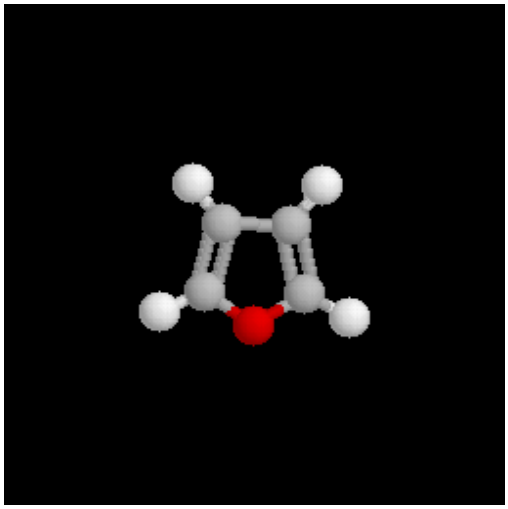
Dioxan,
1,4-dioxane



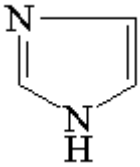


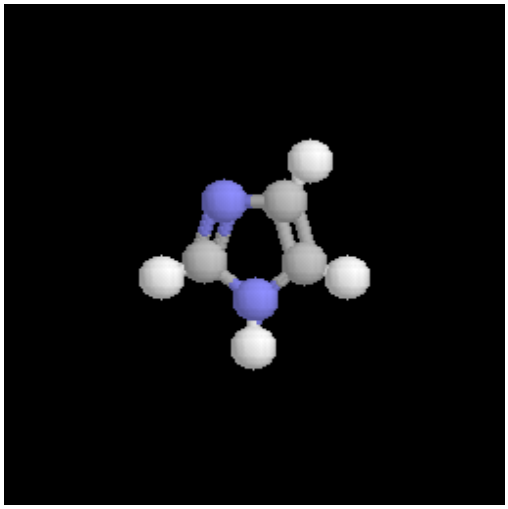
Furan



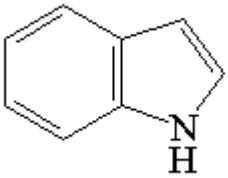


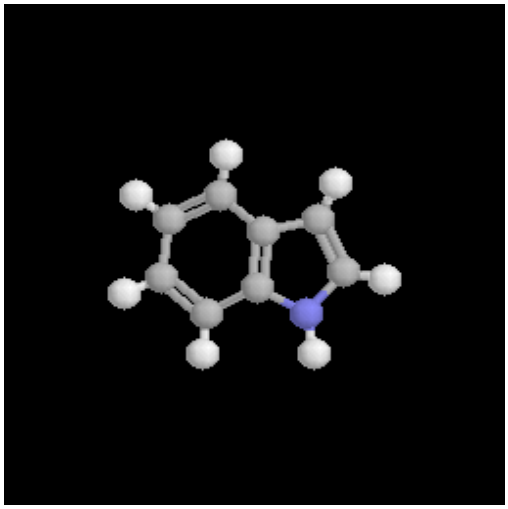
Imidazole



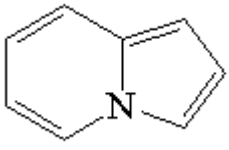


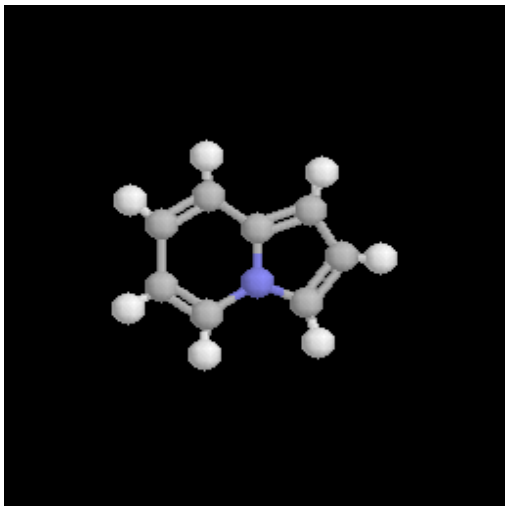
Indole



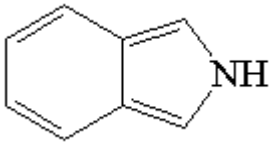


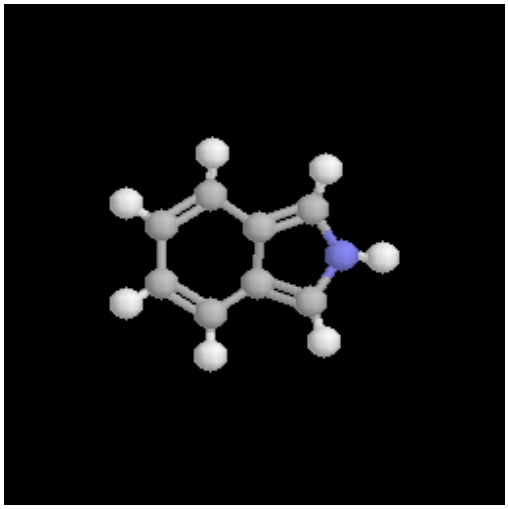
Indolizine



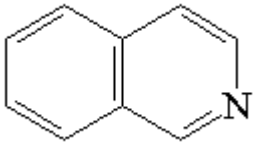


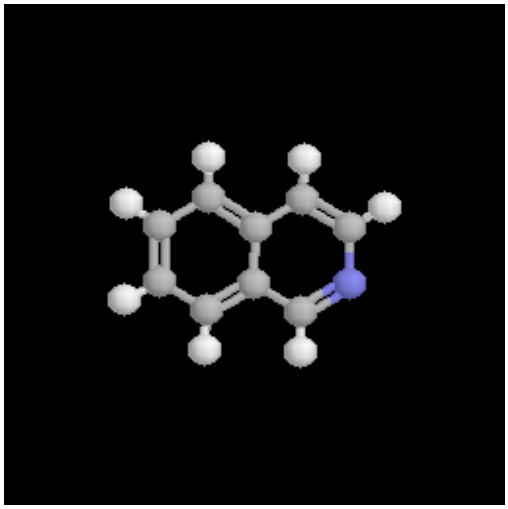
Isoindole



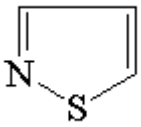


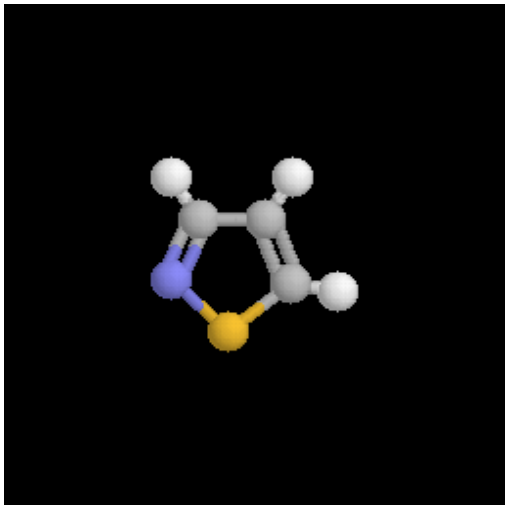
Isoquinoline



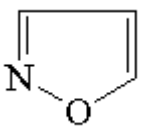


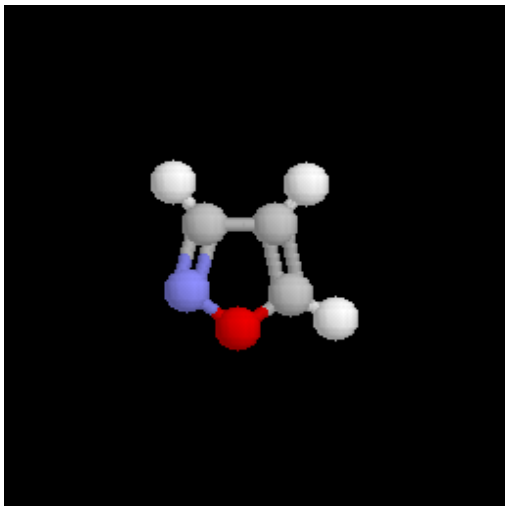
Isothiazole,
1,3-thiazole



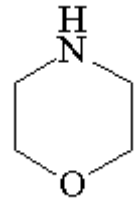


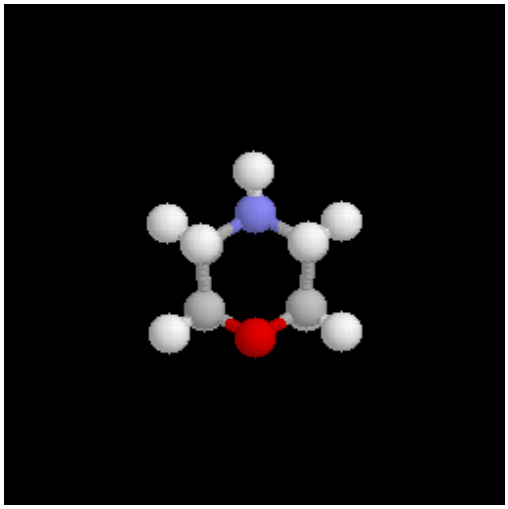
Isoxazole,
4,5-dihydroisoxazole



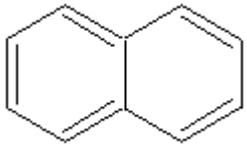


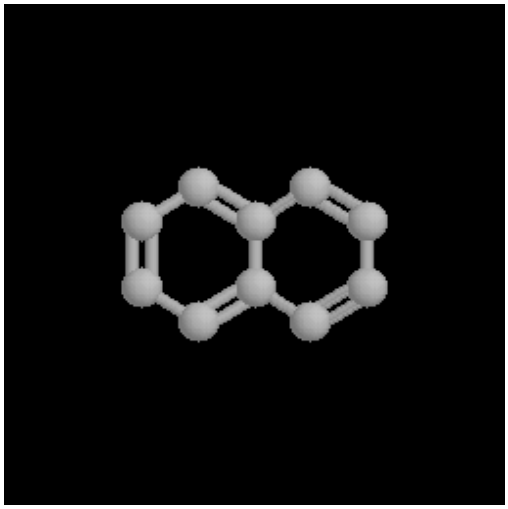
Morpholine



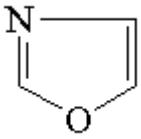


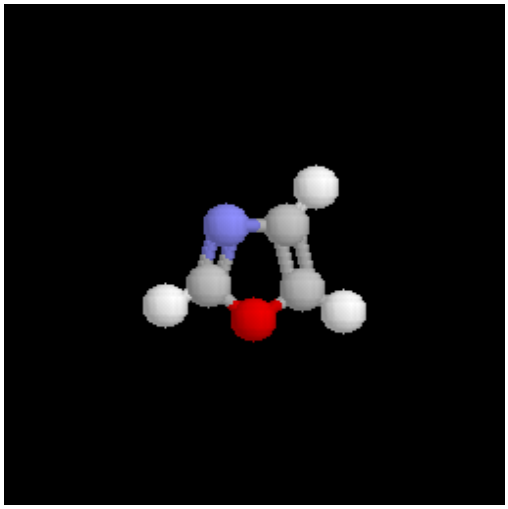
Naphthalene



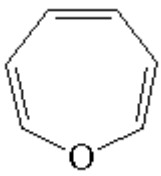


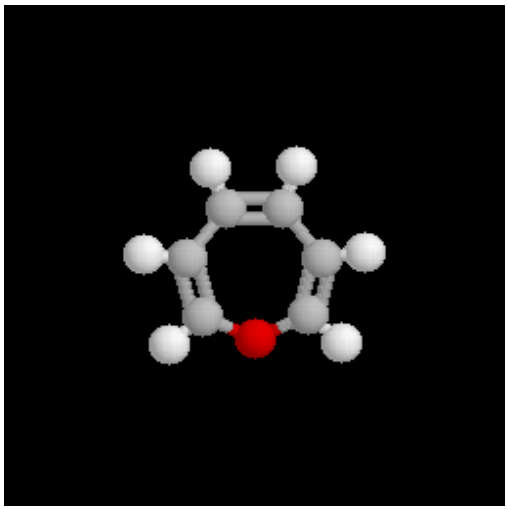
Oxazole,
1,3-oxazole



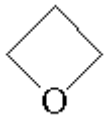


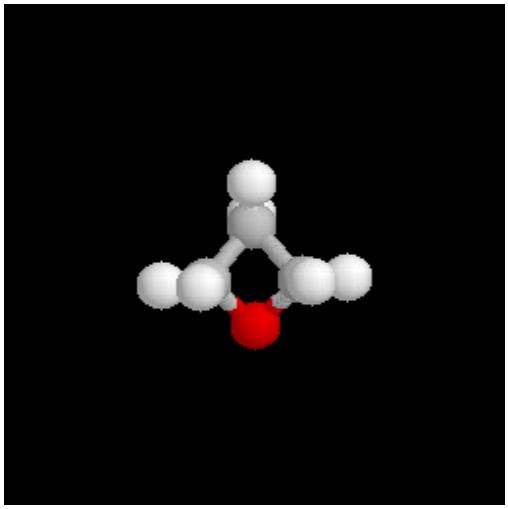
Oxepine



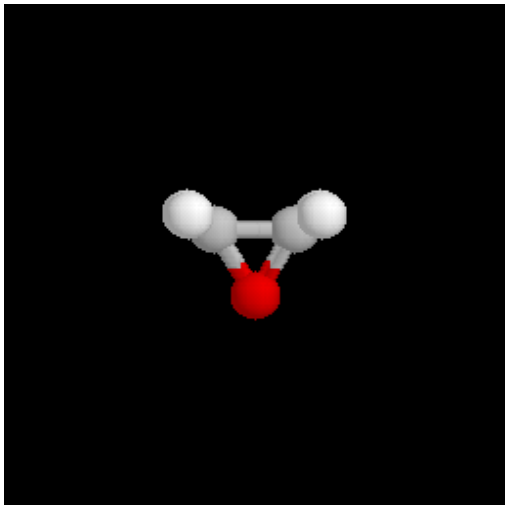


Oxetane

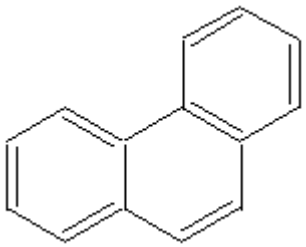


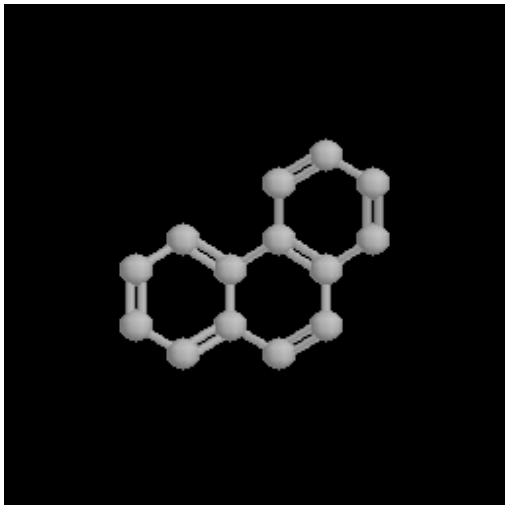


Oxirane (an epoxide)

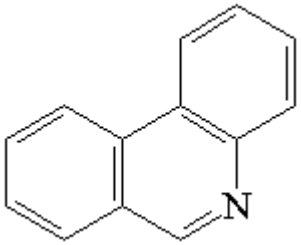


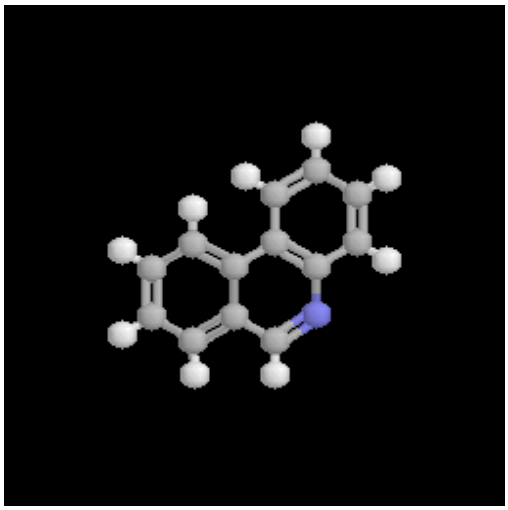
Phenanthrene



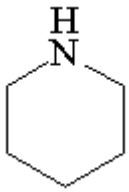


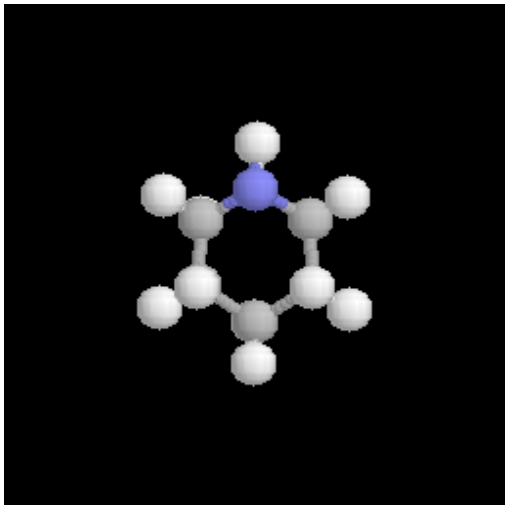
Phenanthridine



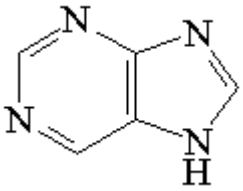


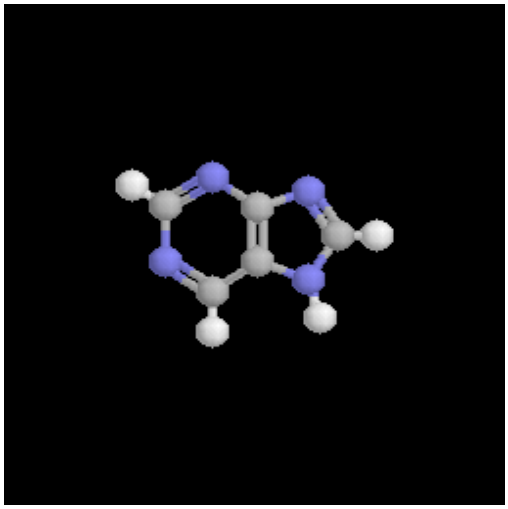
Piperidine



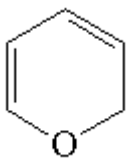


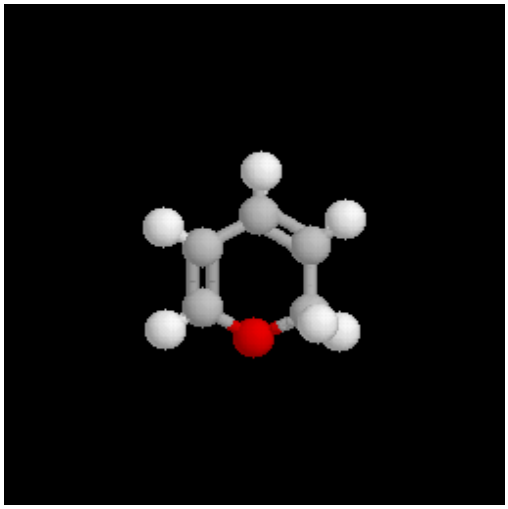
Purine



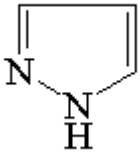


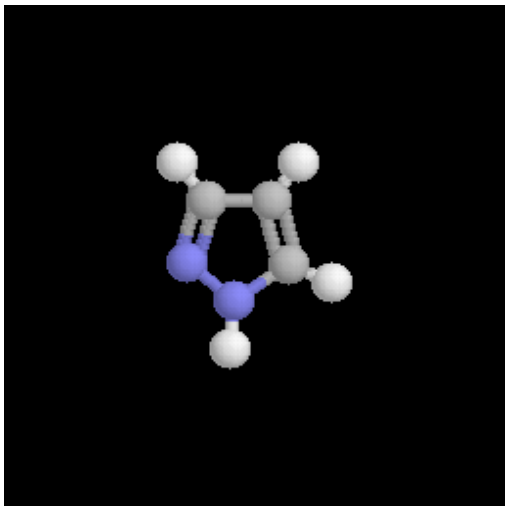
2H-Pyran



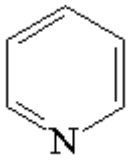


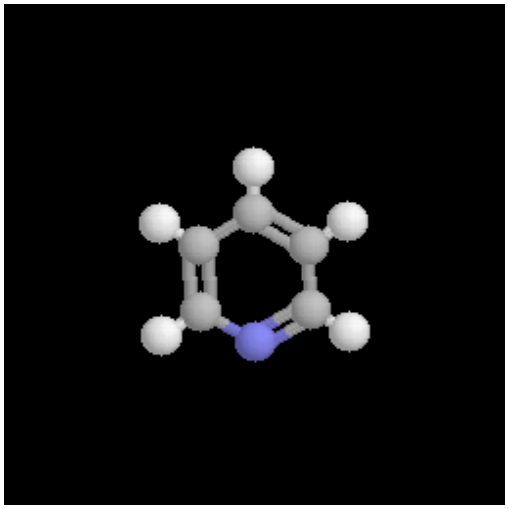
Pyrazole



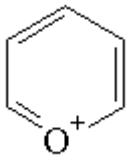


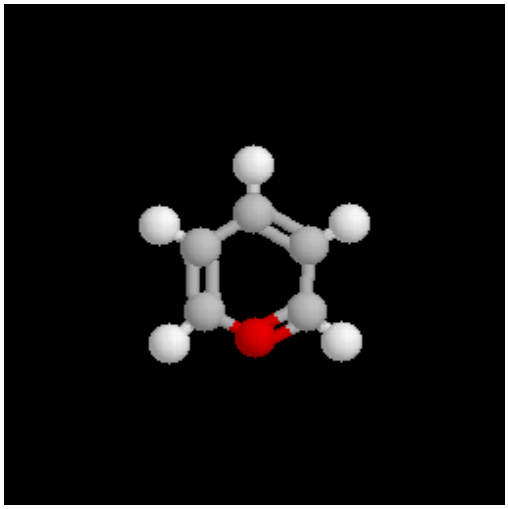
Pyridine



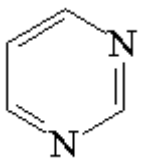


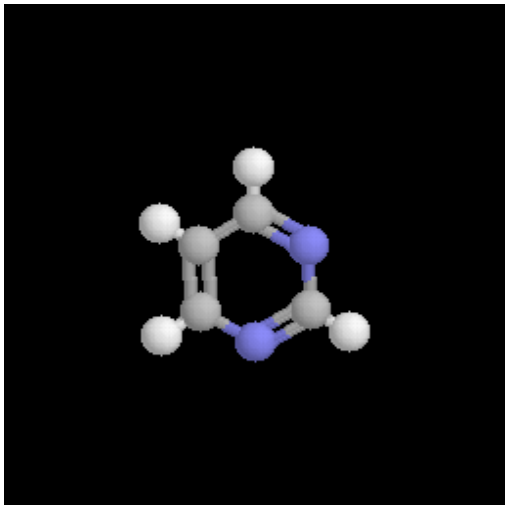
Pyrilium



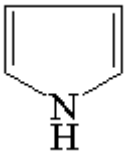


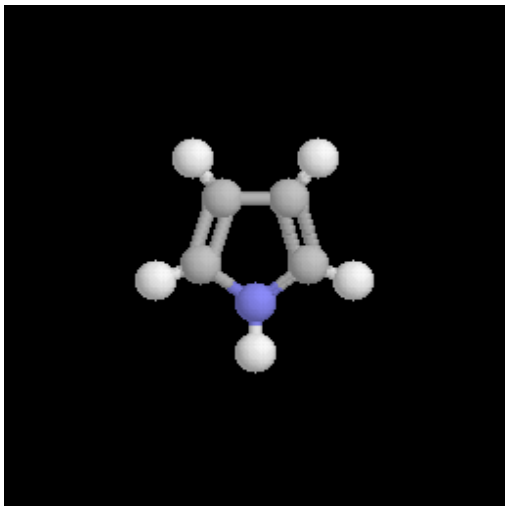
Pyrimidine



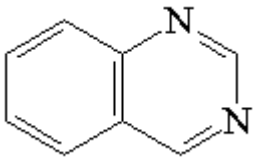


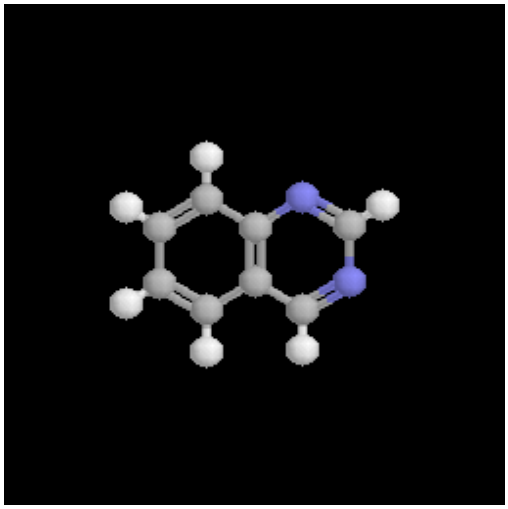
Pyrrole



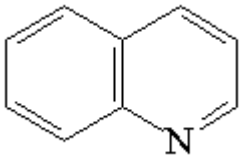


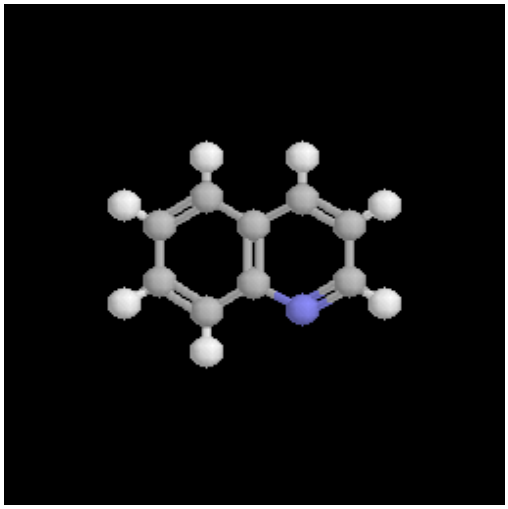
Quinazoline



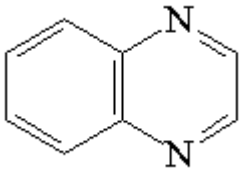


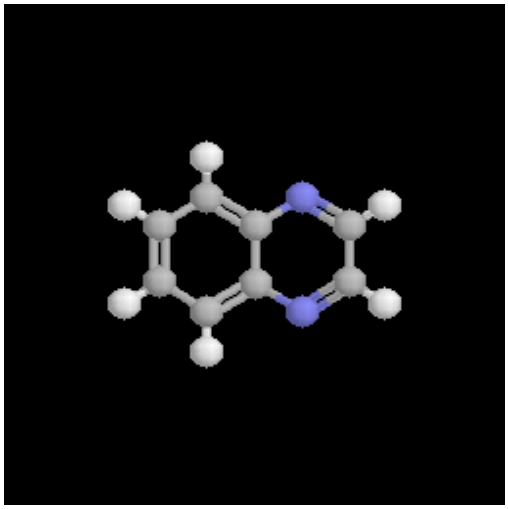
Quinoline



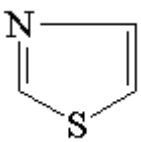


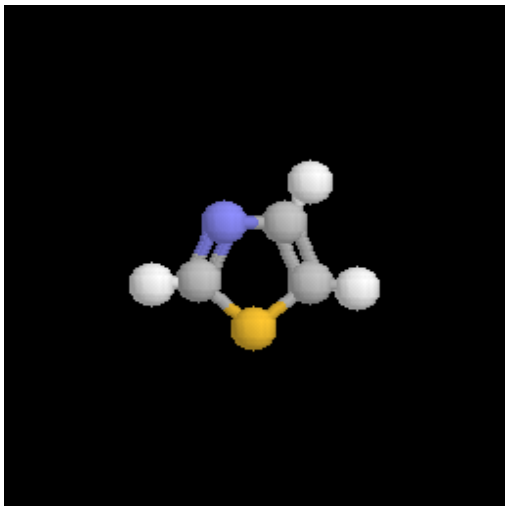
Quinoxaline



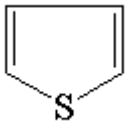


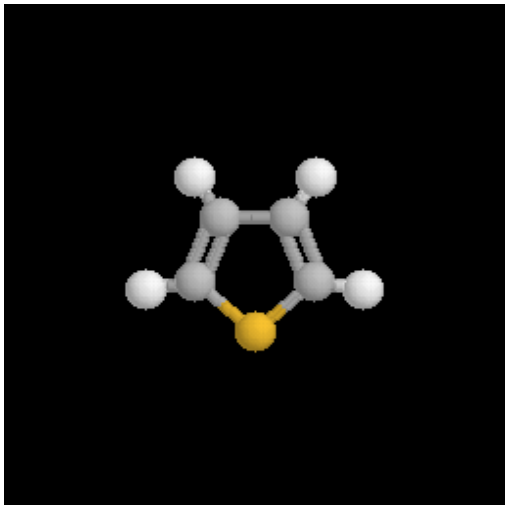
Thiazole





Thiophen

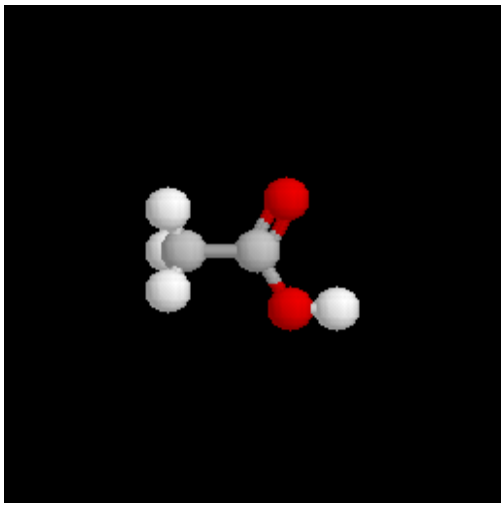
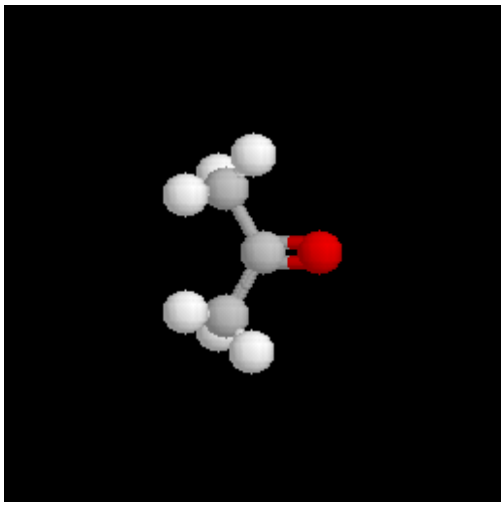
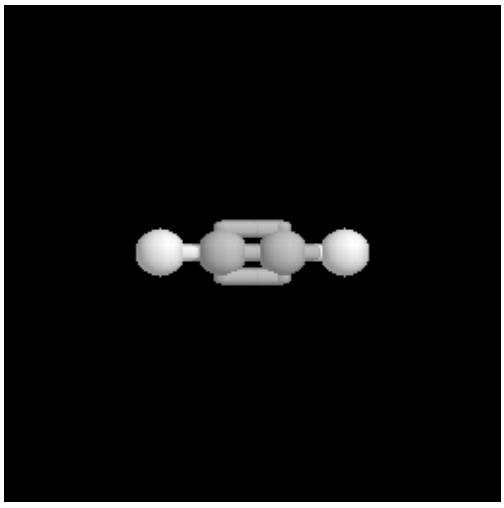


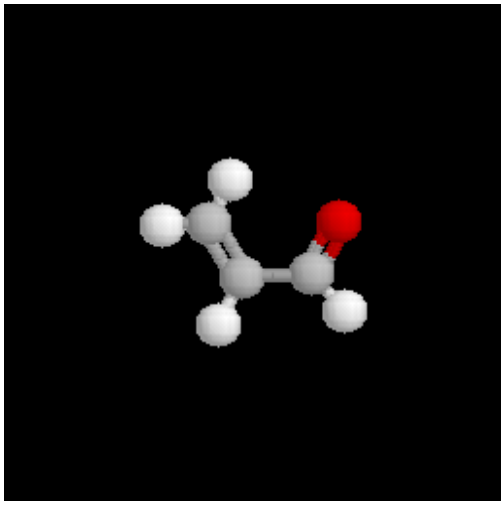
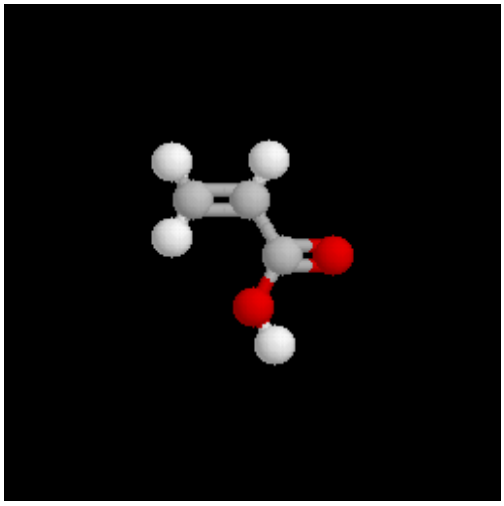
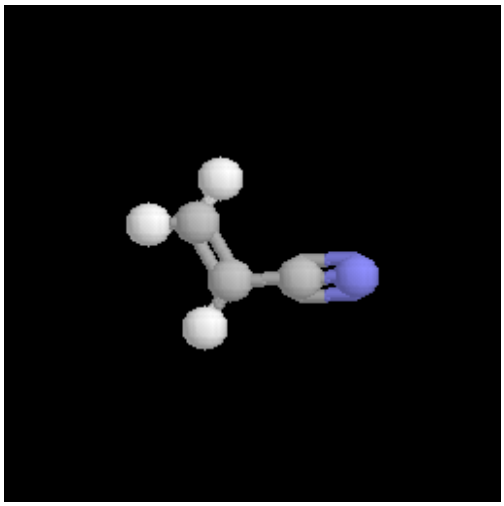
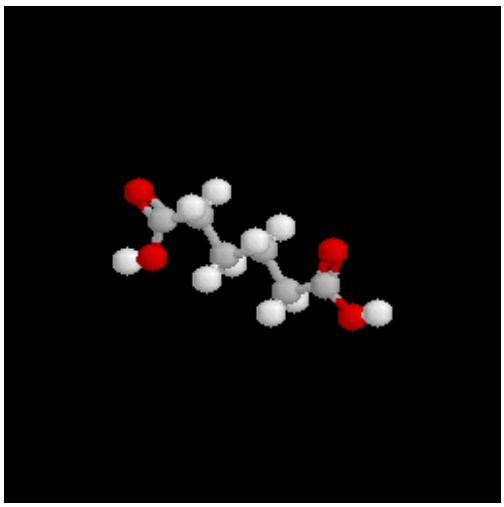


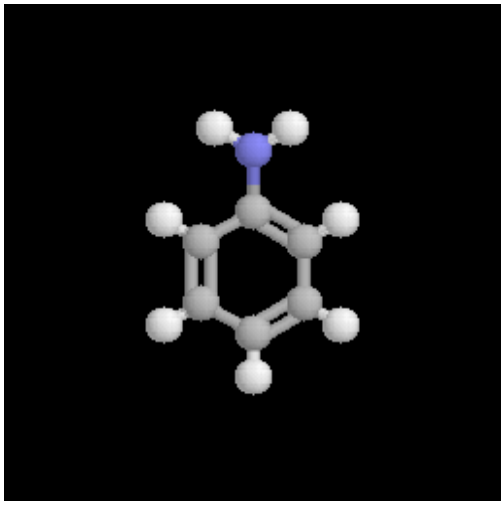
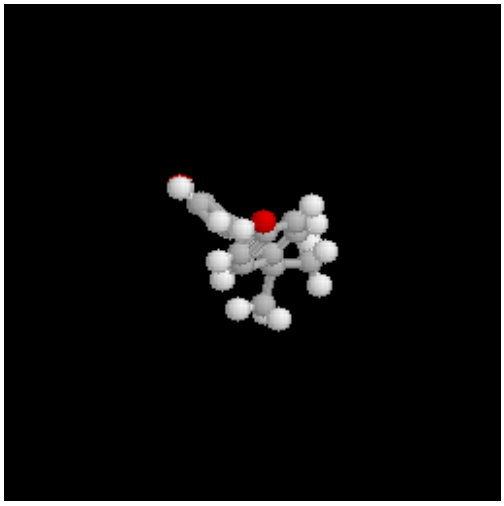
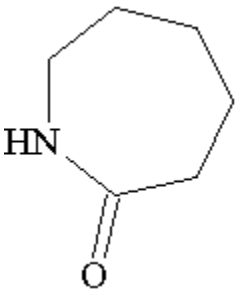
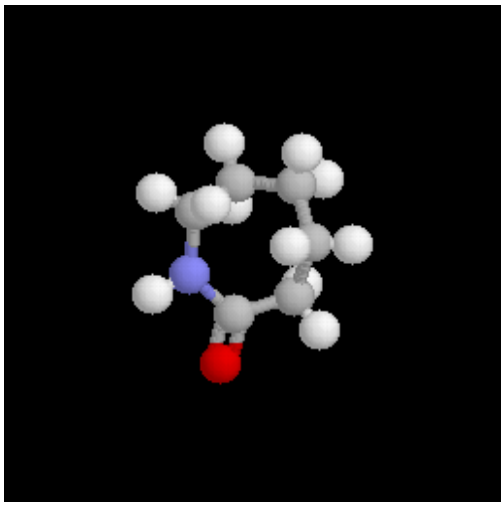
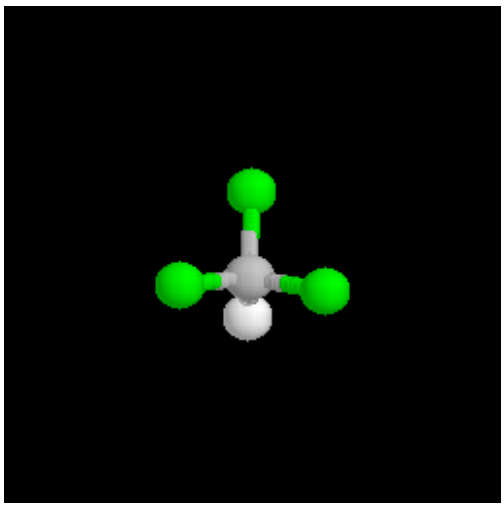
Structures of Selected Organic Compounds

(with standard abbreviations shown in parenthesis)

Instructions

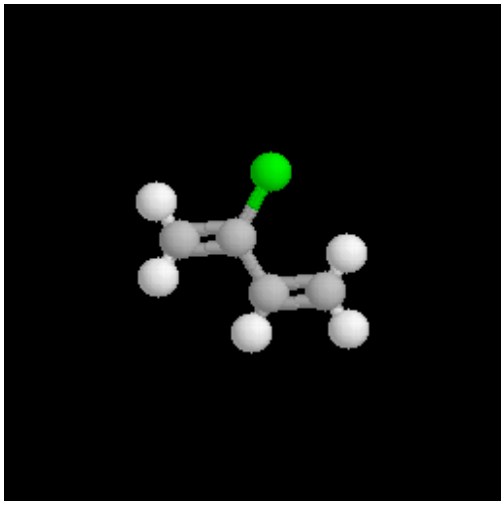
Acetic Acid	$MeCO_2H$	
Acetone	MeCOMe	
Acetylene, Ethyne	HC≡CH	

Acrolein	CH_2=CHCHO	
Acrylic Acid	CH_2=CHCO_2H	
Acrylonitrile	CH_2=CHCN	
Adipic Acid, 1,4-Butanedicarboxylic acid, Hexanedioic acid	$HO_2C(CH_2)_4CO_2H$	

Aniline	$PhNH_2$	
Bisphenol A	$(4\text{-}HOC_6H_4)_2CMe_2$	
e-Caprolactam, Azepan-2-one		
Chloroform, Trichloromethane	$CHCl_3$	

Chloroprene,
2-chlorobuta-1,3-diene

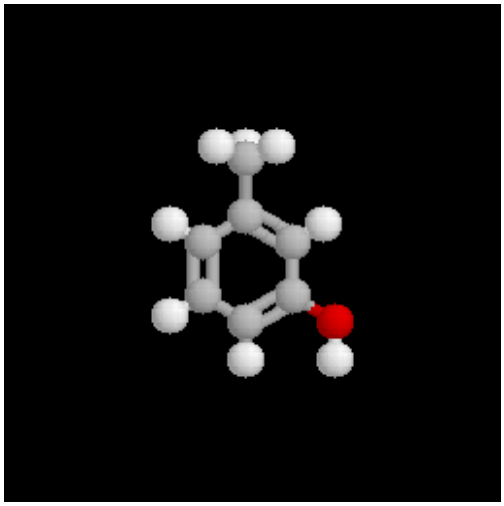
$CH_2=CClCH=CH_2$



m-cresol shown

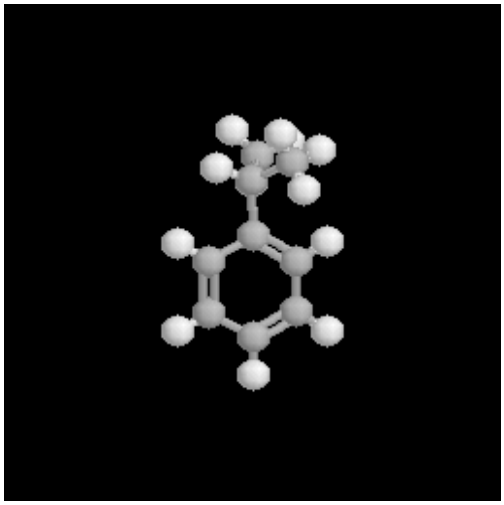
Cresol,
methylphenol

MeC_6H_4OH

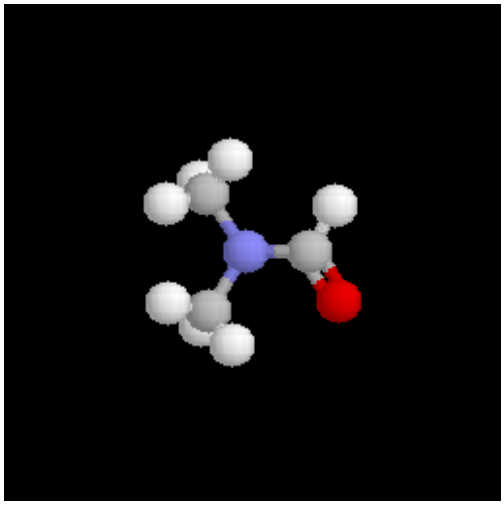


Cumene,
Isopropylbenzene

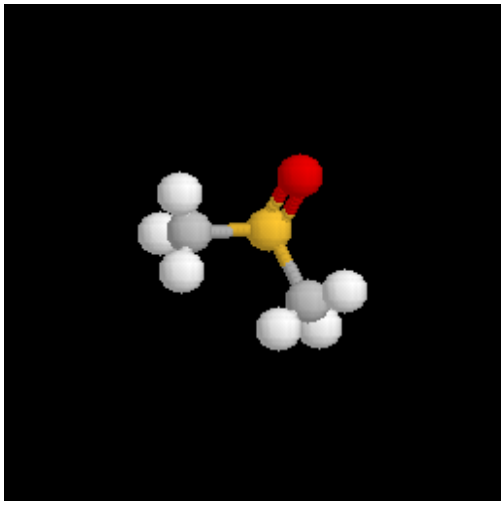
$PhCHMe_2$



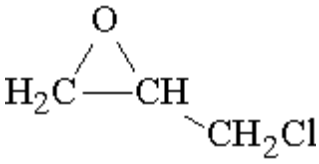
N,N-Dimethylformamide (DMF) Me_2NCHO

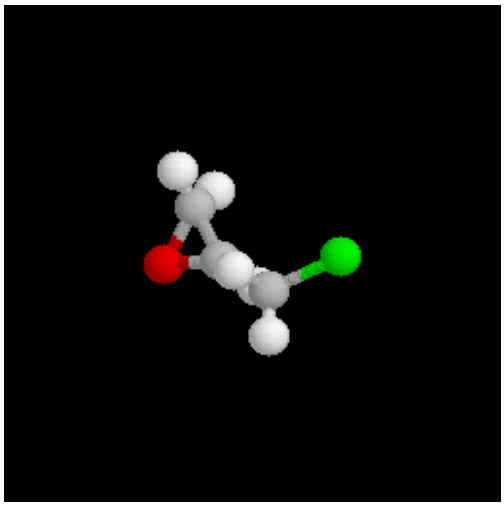


Dimethylsulphoxide, (methylsulfinyl)methane (DMSO) Me_2SO

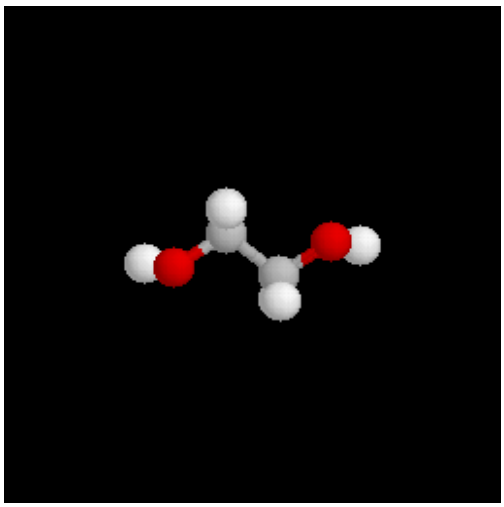


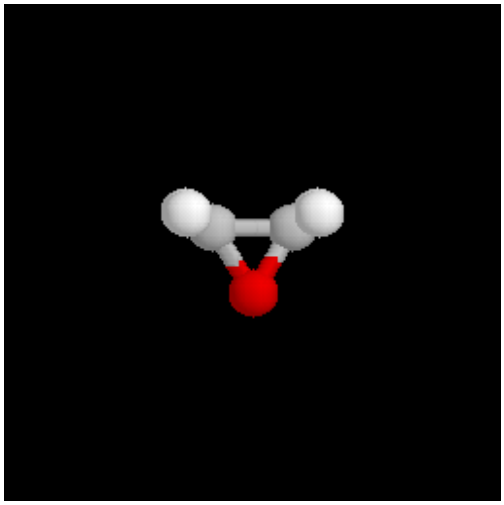
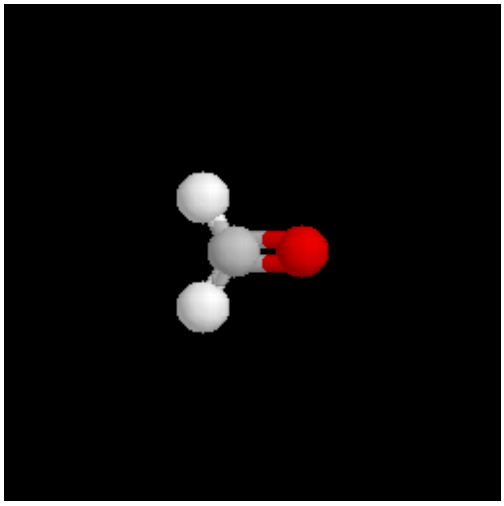
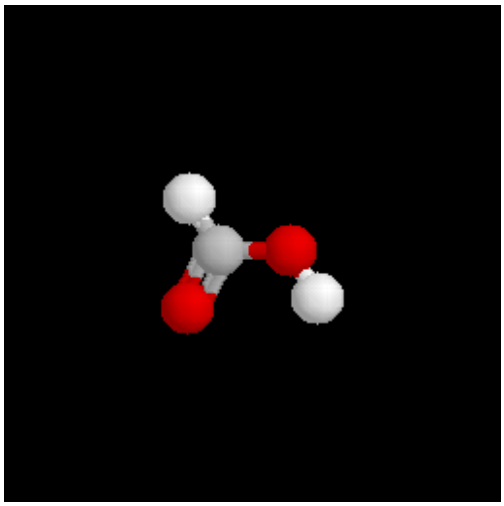
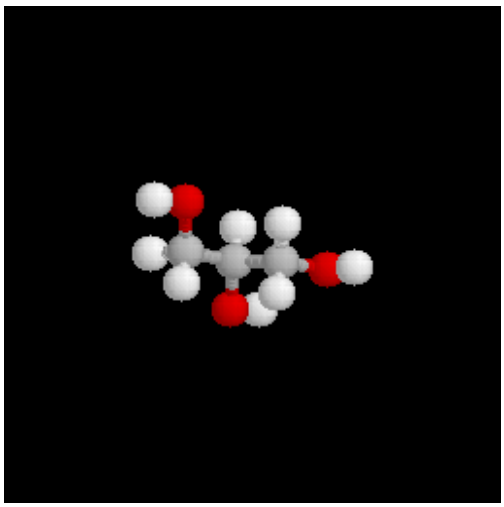
Epichlorhydrin, 2-(chloromethyl)oxirane

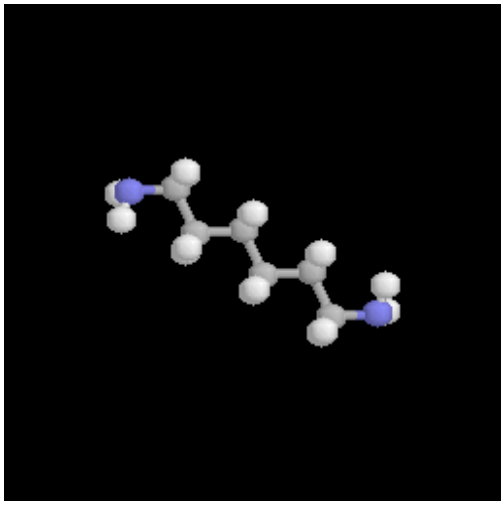
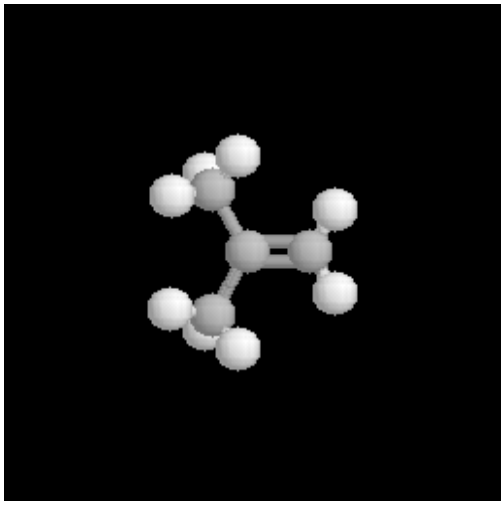
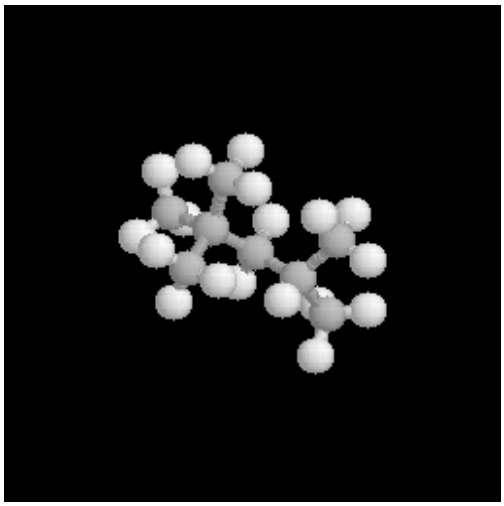
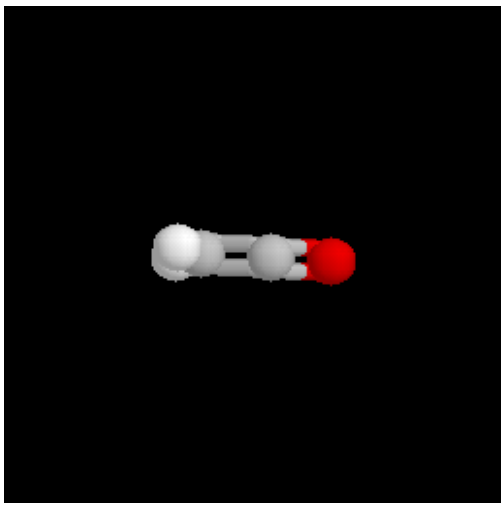


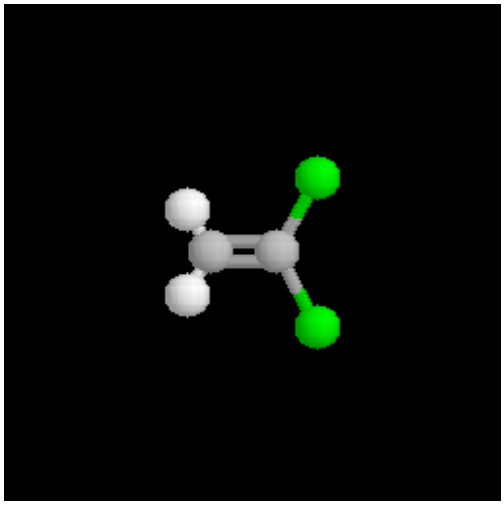
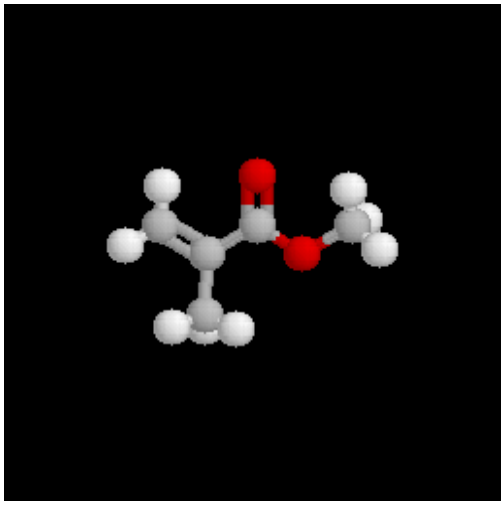
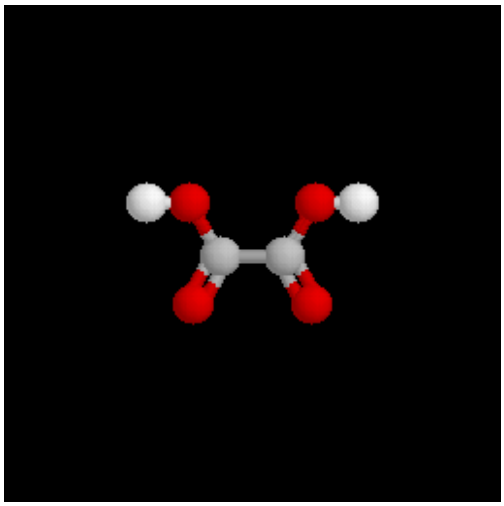


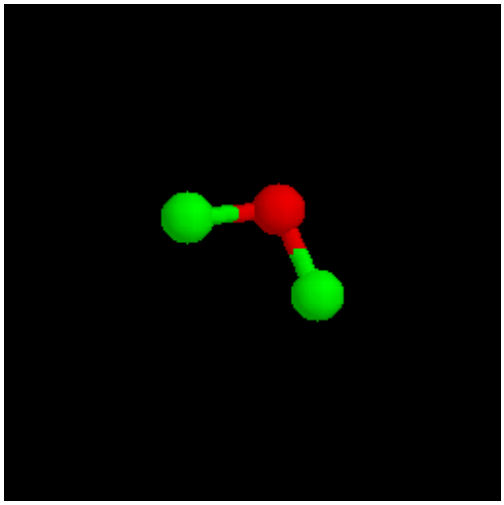
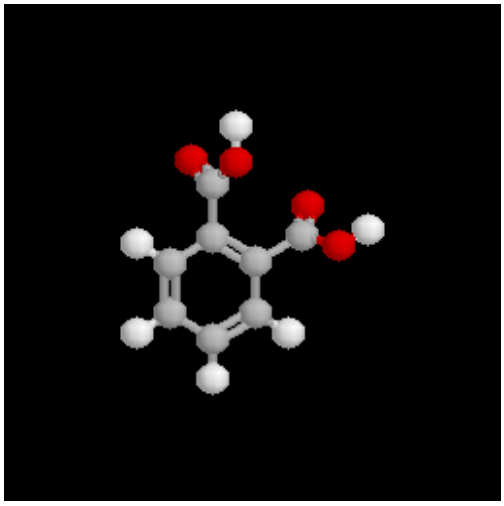
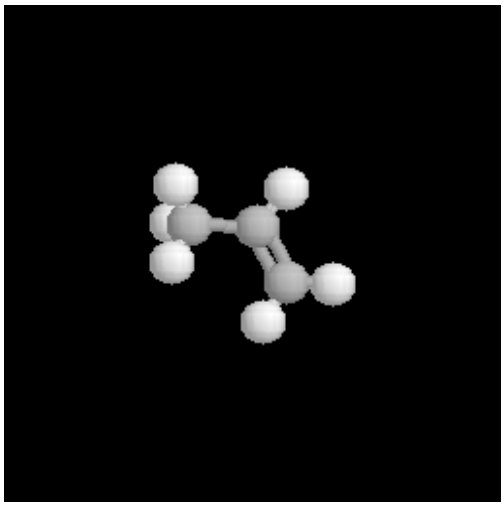
Ethylene Glycol, 1,2-Dihydroxyethane, 1,2-ethanediol $HOCH_2CH_2OH$

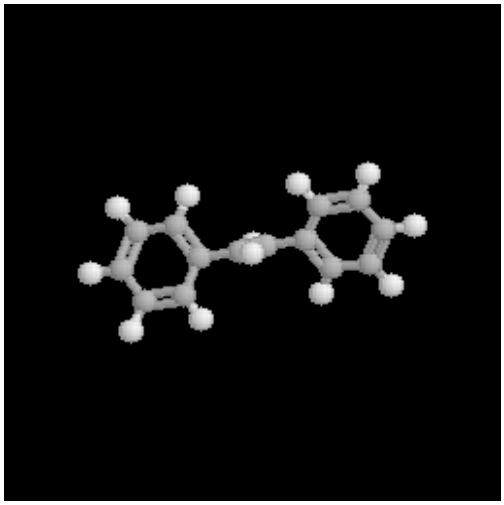
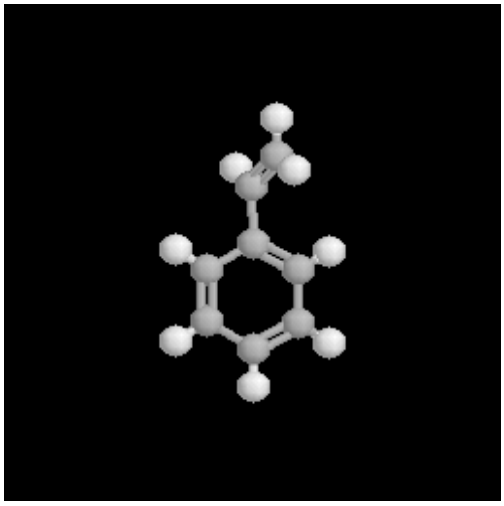
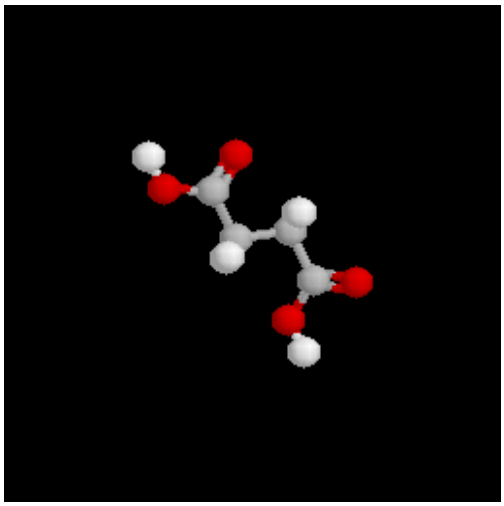
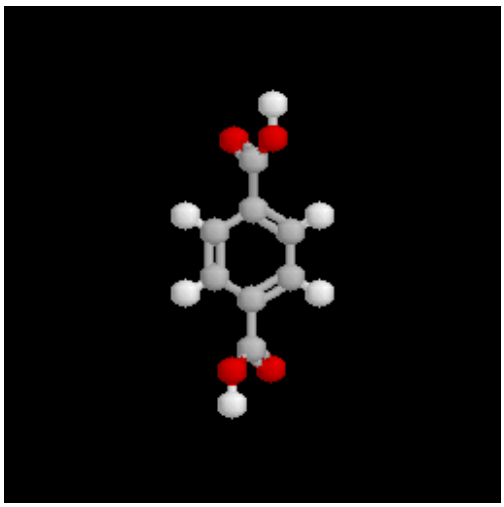


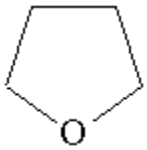
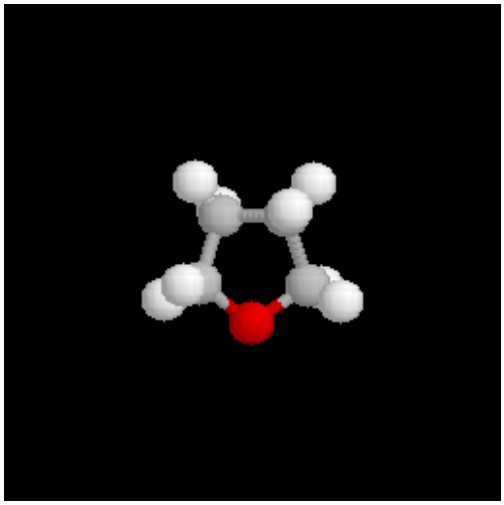
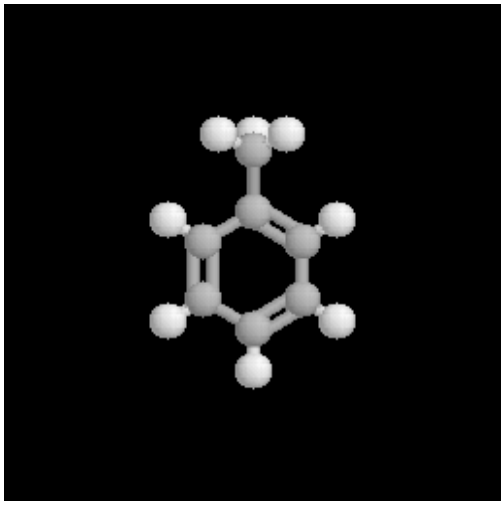
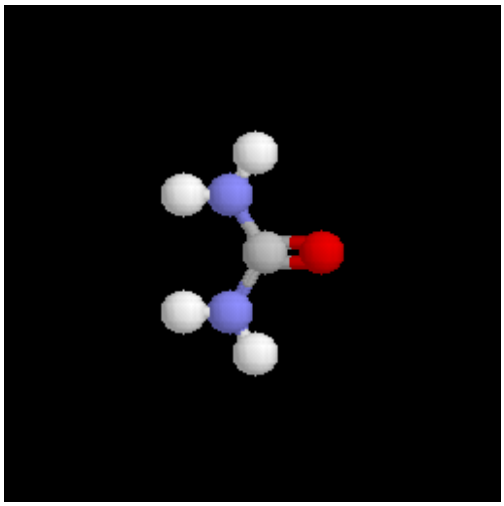
Ethylene oxide, Oxirane		
Formaldehyde, Methanal	CH_2O	
Formic Acid	HCO_2H	
Glycerol, 1,2,3-Propanetriol	$HOCH_2CH(OH)CH_2OH$	

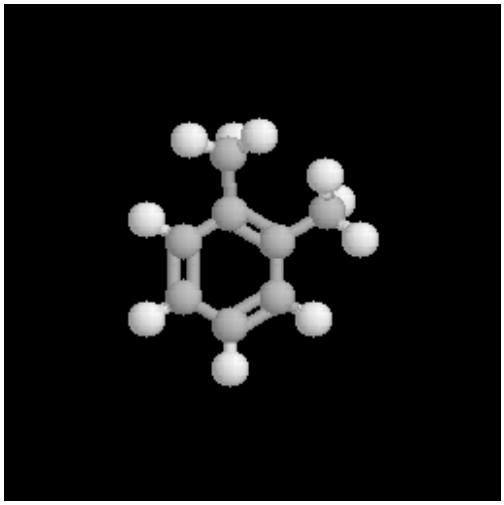
Hexamethylenediamine, 6-aminohexylamine	$H_2N(CH_2)_6NH_2$	
Isobutylene, 2-methylprop-1-ene	$Me_2C{=}CH_2$	
Iso-octane, 2,2,4-trimethylpentane	$Me_3CCH_2CHMe_2$	
Ketene, Ethylenone	$CH_2{=}CO$	

Methylene Dichloride, Dichloromethane	CH_2Cl_2	
Methyl Methacrylate, Methyl 2-methylacrylate	$CH_2=CMeCO_2Me$	
Neoprene	$[–CH_2CCl=CHCH^{2-}]_n$	
Oxalic acid	$HO_2C.CO_2H$	

Phosgene	Cl_2O	
Phthalic acid, Benzene-1,2-dicarboxylic acid	$1,2\text{-}C_6H_4(CO_2)H)_2$	
Propylene, Prop-1-ene	$MeCH{=}CH_2$	
PVC	$[–CH_2CHCl–]_n$	

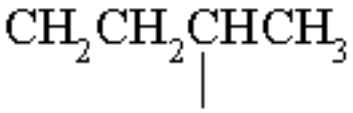
Stilbene, 1,2-Diphenylethylene	PhCH=CHPh	
Styrene, Phenylethylene, Vinyl benzene	$PhCH=CH_2$	
Succinic Acid	$HO_2CCH_2CH_2CO_2H$	
Terephthalic acid, Benzene-1,4-dicarboxylic acid	$1,4\text{-}C_6H_4(CO_2H)_2$	

Tetrahydrofuran	(THF)		
Toluene, Methylbenzene	PhMe		
Urea	H_2NCONH_2		
Xylene, Dimethylbenzene	$C_6H_4Me_2$		*o*-xylene shown



Structures of Selected Organic Groups

with non-standard systematic names (with 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)	
t-Butyl	(Bu^t)	$(CH_3)C_3–$
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 (Ethanoate)	(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		$(C_6H_5)_3C–$

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, 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

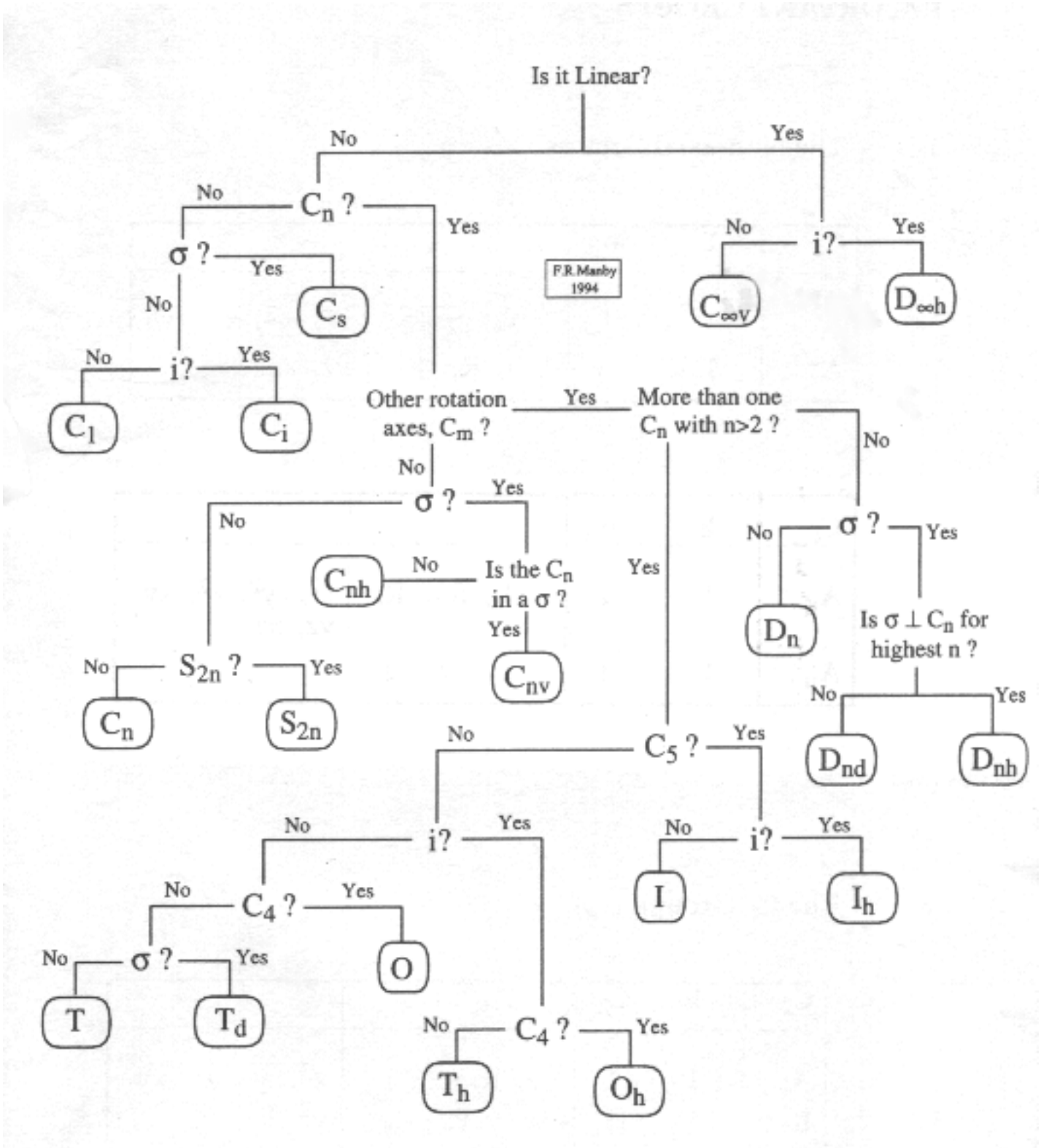
e.g. 2,3,3-trimethylcyclopentanone

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

Arithmetical Progression

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

How to Assign a Molecule to its Point Group



Binomial Series

Definitions

$n! = n(n-1)(n-2)....1 \quad (0!=1)$

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

Binomial Series

$(x + y)^n = x^n + {}^nC_1x^{n-1}y + {}^nC_2x^{n-2}y^2 + ... {}^nC_rx^{n-r}y^r + ... y^n$

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

						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 position 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.

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	σ_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	

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

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**	**$2C_3$**	**$3C_2$**		
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)

The C_{nv} Groups

C_{2v}	E	C_2	σ_v (xz)	σ'_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 cos72°	2 cos144°	0	(x,y)(R_x, R_y)	(xz,yz)
E_2	2	2 cos144°	2 cos72°	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

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	

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
A_u	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**	**$2C_5$**	**$2C^2_5$**	**$5C_2$**	**σ_h**	**$2S_5$**	**$2S^3_5$**	**$5\sigma_v$**		
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	$2\cos72^o$	$2\cos144^o$	0	2	$2\cos72^o$	$2\cos144^o$	0	(x, y)	
E'_2	2	$2\cos144^o$	$2\cos72^o$	0	2	$2\cos144^o$	$2\cos72^o$	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	$2\cos72^o$	$2\cos144^o$	0	-2	$-2\cos72^o$	$-2\cos144^o$	0	(R_x, R_y)	(xy, yz)
E''_2	2	$2\cos144^o$	$2\cos72^o$	0	-2	$-2\cos144^o$	$-2\cos72^o$	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		

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, $z(x^2 - y^2)$][$x(x^2 + y^2)$]

D_{4d}	E	$2S_8$	$2C_4$	$2S^3_8$	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	$2^{1/2}$	0	$-2^{1/2}$	-2	0	0	(x, y)	
E_2	2	0	-2	0	2	0	0		(x^2 - y^2, xy)
E_3	2	$-2^{1/2}$	0	$-2^{1/2}$	-2	0	0	(R_x, R_y)	(xz, yz)

D_{5d}	**E**	**$2C_5$**	**$2C^2_5$**	**$5C'_2$**	**i**	**$2S^3_{10}$**	**$2S_{10}$**	**$5\sigma_d$**		
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 cos72º	2 cos144º	0	2	2 cos72º	2 cos144º	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	2 cos144º	2 cos72º	0	2	2 cos144º	2 cos72º	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 cos72º	2 cos144º	0	-2	-2 cos72º	-2 cos144º	0	(x, y)	
E_{2u}	2	2 cos144º	2 cos72º	0	-2	-2 cos144º	-2 cos72º	0		

The Cubic Groups

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	$8C_3$	$6C_2$	$6C_4$	$3C_2 (C^2_4)$	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, Rz)		
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)]

The Continuous Groups

$C_{\infty v}$	E	$2C^{\phi}_{\infty}$	…	$\infty\sigma_v$		
$A_1 \equiv \Sigma^+$	1	1	…	1	z	$x^2 + y^2, z^2$
$A_2 \equiv \Sigma^-$	1	1	…	-1	R_z	
$E_1 \equiv \Pi$	2	$2\cos\Phi$	…	0	$(x,y)(R_x, R_y)$	(xz, yz)
$E_2 \equiv \Delta$	2	$2\cos2\Phi$	…	0		$(x^2 - y^2, xy)$
$E_2 \equiv \Phi$	2	$2\cos3\Phi$	…	0		
…	…	…	…	…		

$D_{\infty h}$	E	$2C^{\phi}_{\infty}$	…	$\infty\sigma_v$	i	S^{ϕ}_{∞}	…	$\infty C'_2$		
$A_{1g} \equiv \Sigma^+_g$	1	1	…	1	1	1	…	1		$x^2 + y^2, z^2$
$A_{2g} \equiv \Sigma_g$	1	1	…	-1	1	1	…	-1	R_z	
$E_{1g} \equiv \Pi_g$	2	$2\cos\Phi$	…	0	2	$-2\cos\Phi$	…	0	(R_x, R_y)	(xz,yz)
$E_{2g} \equiv \Delta_g$	2	$2\cos2\Phi$	…	0	2	$2\cos2\Phi$	…	0		$(x^2 - y^2, xy)$
...	…	…	…	…	…	…	…	…		
$A_{1u} \equiv \Sigma^+_u$	1	1	…	1	-1	…	…	-1	z	
$A_{2u} \equiv \Sigma^-_u$	1	1	…	-1	-1	-1	…	1		
$E_{1u} \equiv \Pi_u$	2	$2\cos\Phi$	…	0	-2	$2\cos\Phi$	…	0	(x, y)	

$\mathbf{E_{2u} \equiv \Delta_u}$	2	2cos2Φ	…	0	-2	-2 cos2Φ	…	0		
…	…	…	…	…	…	…	…	…		

Complex Numbers

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

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

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

v_2/ v_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

---

v_1 = number of degrees of freedom of the numerator and v_2 = number of degrees of freedom of the denominator

Derivatives and Indefinite Integrals of Elementary Functions

f(x)	$f'(x) = \frac{df(x)}{dx}$	$F(x) = \int f(x)dx$
x^n	$nx^{n-1}(n \neq 0)$	$x^{n+1}/(n+1)(n \neq -1)$ $\ln x\ (n = -1)$
$\ln x$	$1/x$	$x \ln x - x$
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
$\sec^2 x$	$2 \sec^2 x \tan x$	$\tan x$
$\frac{1}{(a^2 - x^2)^{1/2}}$	$x(a^2 - x^2)^{-3/2}$	$\sin^{-1}(x/a),\ \|x\|<a$
$\tan x$	$\sec^2 x$	$-\ln \|\cos x\|$

Descent In Symmetry for Selected Groups

1 General Notes

These tables show the correlation between (irreducible) representations of a group and those of some of its subgroup (in many cases the parent group has more subgroups than the ones shown).

Where there are various possibilities for the mapping of σ and C_2 elements from the parent group to one of its subgroups these are indicated in the heading.

2 The C_{nv} Groups

C_{2v}	C_2	$C_s\sigma$ (zx)	$C_s\,\sigma$ (yz)
A_1	A	A'	A'
A_2	A	A''	A''
B_1	B	A'	A''
B_2	B	A''	A'

C_{3v}	C_s
A_1	A'
A_2	A''
E	$A' + A''$

C_{4v}	C_{2v} σ_v	C_{2v} σ_d
A_1	A_1	A_1
A_2	A_2	A_2

B_1	A_1	A_2
B_2	A_2	A_1
E	$B_1 + B_2$	$B_1 + B_2$

3 The D_{nh} Groups

D_{3h}	C_{3v}	C_{2v} $\sigma_h \rightarrow \sigma_v$	C_s σ_h	C_s σ_v
A_1'	A_1	A_1	A'	A'
A_2'	A_2	B_2	A'	A''
E	E	$A_1 + B_2$	$2A'$	$A' + A'$
A_1''	A_2	A_2	A''	A''
A_2''	A_1	B_1	A''	A'
E''	E	$A_2 + B_1$	$2A''$	$A' + A'$

D_{4h}	$D_{2d}C'_2$ $(\rightarrow C'_2)$	$D_{2d}C''_2$ $(\rightarrow C'_2)$	$D_{2h}C'_2$	$D_{2h}C''_2$	$D_2C'_2$	$D_2C''_2$	C_{4h}	C_{4v}	$C_{2v}C_2$, σ_v	$C_{2v}C_2$, σ_d
A_{1g}	A_1	A_1	A_g	A_g	A	A	A_g	A_1	A_1	A_1
A_{2g}	A_2	A_2	B_{1g}	B_{1g}	B_1	B_1	A_g	A_2	A_2	A_2
B_{1g}	B_1	B_2	A_g	B_{1g}	A	B_1	B_g	B_1	A_1	A_2
B_{2g}	B_2	B_1	B_{1g}	A_g	B_1	A	B_g	B_2	A_2	A_1
E_g	E	E	$B_{2g} + B_{3g}$	$B_{2g} + B_{3g}$	$B_2 + B_3$	$B_2 + B_3$	E_g	E	$B_1 + B_2$	$B_1 + B_2$
A_{1u}	B_1	B_1	A_u	A_u	A	A	A_u	A_2	A_2	A_2
A_{2u}	B_2	B_2	B_{1u}	B_{1g}	B_1	B_1	A_u	A_1	A_1	A_1

B_{1u}	A_1	A_2	A_u	B_{1g}	A_1	B_1	B_u	B_2	A_2	A_1
B_{2u}	A_2	A_1	B_{1u}	A_u	B_1	A	B_u	B_1	A_1	A_2
E_u	E	E	B_{2u} + B_{3u}	B_{2u} + B_{3u}	B_2 + B_3	B_2 + B_3	E_u	E	$B_1 + B_2$	$B_1 + B_2$

4 The Cubic Groups

T_d	D_{2d}	C_{3v}	C_{2v}
A_1	A_1	A_1	A_1
A_2	B_1	A_2	A_2
E	A_1 + B_1	E	$A_1 + A_2$
T_1	A_2 + E	A_2 + E	$A_2 + B_1$ + B_2
T_2	B_2 + E	A_1 + E	$A_1 + B_2$ + B_1

O_h	T_d	D_{4h}	D_{3d}
A_{1g}	A_1	A_{1g}	A_{1g}
A_{2g}	A_2	B_{1g}	A_{2g}
E_g	E	A_{1g} + B_{1g}	E_g
T_{1g}	T_1	$A_{2g} + E_g$	A_{2g} + E_g
T_{2g}	T_2	$B_{2g} + E_g$	A_{1g} + E_g
A_{1u}	A_2	A_{1u}	A_{1u}
A_{2u}	A_1	B_{1u}	B_{1u}
E_u	E	A_{1u} + B_{1u}	E_u

T_{1u}	T_2	$A_{2u} + E_u$	$A_{2u} + E_u$
T_{2u}	T_1	$B_{2u} + E_u$	$A_{1u} + E_u$

Direct Product Rules for Chemically Important Groups

1. **General Rules**

×	′	″
′	′	″
′	″	′
″	′	′

×	g	u
g	g	u
u	u	g

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

×	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}**

×	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_2	A_1	B_2	B_1	E_1	E_2
B_1	B_1	B_2	A_1	A_2	E_2	E_1
B_2	B_2	B_1	A_2	A_1	E_2	E_1

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

3. **For D_2, D_{2h}**

×	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}**

×	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}**

×	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**

×	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 $C_{\infty}v$, $D_{\infty}h$**

×	Σ^+	Σ^-	Π	Δ	…
Σ^+	Σ^+	Σ^-	Π	Δ	
Σ^-		Σ^+	Π	Δ	
Π			$\Sigma^+ + [\Sigma^-] + \Delta$	$\Pi + \Phi$	
Δ				$\Sigma^+ + [\Sigma^-] + G$	
:					

Geometrical Progression

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

Group Theoretical Formulae

1. A reducible representation, Γ, associated with a group of g symmetry operations, R, contains a given irreducible representation Γ_i, n_i times, where

$$n_i = \frac{1}{g}\sum_{R} \chi_i(R)\chi(R)$$

2. The quantity f(R) is the contribution to the character of the Cartesian representation by *each* atom *un*shifted by an operation.

Operation	f(R)	Operation	f(R)
E	3	S_3	-2
σ	1	S_4	-1
i	-3	S_5	γ-2
C_2	-1	S_5^3	-1-γ
C_3	0	S_5^7	-1-γ
C_4	1	S_5^9	γ-2
C_5	γ	S_6	0
C_5^2	1-γ		
C_5^3	1-γ	C_n^K	1 + 2cos(2π k/n)
C_6	2	S_n^k	-1 + 2cos(2π k/n)

Hyperbolic Functions

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

$\sinh x = \frac{1}{2}(e^x - e^{-x})$

$\tanh x = \frac{\sinh x}{\cosh x}$

$\cosh^2 x - \sinh^2 x = 1$

$\cosh^2 x + \sinh^2 x = \cosh 2x$

$2 \sinh x \cosh x = \sinh 2x$

$\cosh(-x) = \cosh x$

$\sinh(-x) = -\sinh x$

Integration by Parts

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

MacLaurin Series

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

Normal Distribution (Single-Sided)

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

Deviate μ	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	.3346	.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	.1600	.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	.1351	.1112	.1093	.1075	.1056	.1038	.1020	.1003	.0985
1.3	.0968	.0951	.0934	.0918	.0901	.0858	.0869	.0853	.0838	.0823
1.4	.0808	.0793	.0778	.0764	.0749	.0735	.0721	.0708	.0694	.0681
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

Normal Distribution (Single-Sided)

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									
	0.00		0.02		0.01		0.06		0.08	

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	7.85	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**

Quadratic Equations

$ax^2 + bx + c = 0$ has roots. $x = -\frac{b}{2a} \pm \frac{1}{2a}(b^2 - 4ac)^{1/2}$ for real a, b, c.

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

Rules for Differentiation

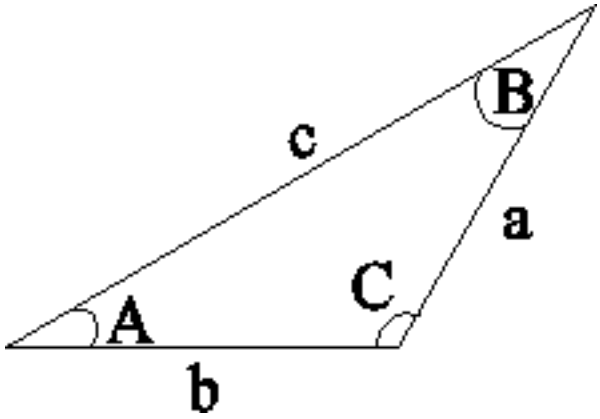
$$\frac{d}{dx}(fg) = f'fg'$$

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

Scalar, Vector Products

$a \cdot b = |a||b| \cos C$

$a \times b = |a||b| \sin C\hat{n}$



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

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

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

Simpson's Rule

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

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

Student's 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	3.044	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.

Taylor Series

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

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

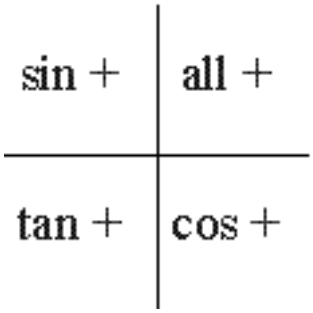
Trapezoidal Rule

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

where h = (b-a)/n

Trigonometrical Formulae

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



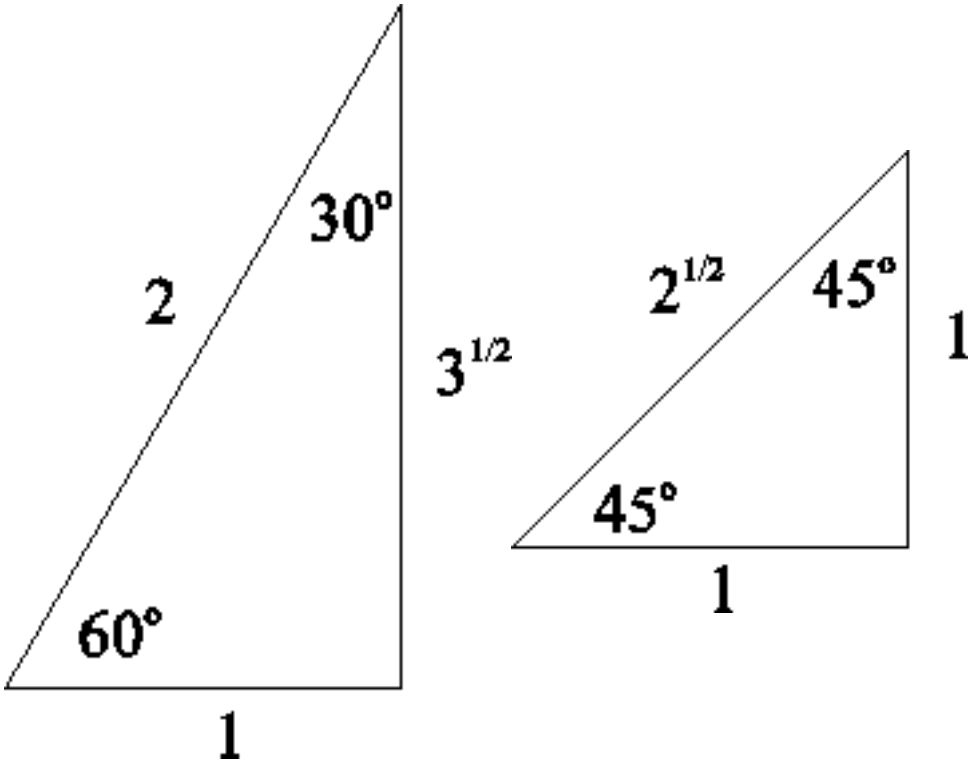
all = sin, tan, cos (π radians = 180º)

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

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

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

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



$\cos^2 x + \sin^2 x = 1$ $\quad \cos(x \pm y) = \cos x \cos y \mp \sin x \sin y$

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

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

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

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

$\sin 2x = 2 \sin x \cos x$ $\quad \cos 3x = 4 \cos^3 x - 3 \cos x$

$\sin 3x = 3 \sin x - 4 \sin^3 x$ $\quad \tan(x \pm y) = \dfrac{\tan x \pm \tan y}{1 \pm \tan x \tan y}$

Atomic Units

Physical Quantity	Symbol	Value
Length	a_0	5.2918×10^{-11} m
Energy	E_h	4.3597×10^{-18} J
Dipole moment	ea_0	8.4784×10^{-30} C m

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_0	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	$\varepsilon_0 = 1/\mu_0 c^2$	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	$R_\infty = me^4\mu_0^2c^3/8h^3$	$1.097\,373 \times 10^{7}$ 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}

ln 10 = 2.3026

ln x = 2.3026 log x

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

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

SI Units

Quantity	Unit Name	Name Symbol
Length	meter	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	N m^{-2} ≡ Pa (Pascal)		1 atmos = 1.013 × 10^5 Pa
	torr (mm Hg)	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}	
Magnetic 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}