Table 4.9. (Continued)

para	1225-1175	1219	*p*-Xylene
	1125-1090	1120	
	1070-1000	1043	
	855-790	796 (s)	
Tri-substitution			
1,2,3-	1175-1125	1162	1,2,3-Trimethylbenzene
	1110-1070	1095	
	1000-960	1009	
	800-755	765 (s)	
	740-695	710 (s)	
1,2,4-	1225-1175	1156	1,2,4-Trimethylbenzene
	1130-1090	1130	
	1000-960	1000	
	900-865	873 (s)	
	855-800	805 (s)	
1,3,5-	1175-1125	1165	1,3,5-Trimethylbenzene
	1070-1000	1039	
	860-810	836 (s)	
	705-685	690 (s)	

Table 4.10. Alcohol Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
ALCOHOLS			
General			
OH unbridged group	3650-3590 sp		
OH inter- and intra-molecularly H - bonded	3570-3450		
OH intermolecularly H-bonded	3400-3200 br		
Primary alcohols			
	1350-1260	1339	
	1065-1020	1028	1-Pentanol
Secondary alcohols			
	1370-1260	1369	
	1120-1080	1111	2-Pentanol
Tertiary alcohols			
	1410-1310	1379	
	1170-1120	1124	2-Methylbutanol
Aromatic ring hydroxy compounds			
OH unbrided	3617-3599 sp		
OH dimer	3460-3322 br		
OH polymer	3370-3322 br		
	1410-1310	1350	
	1225-1175	1225	Phenol

Table 4.11. Peroxide Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
PEROXIDES			
Aliphatic			
	1820-1810		
	1800-1780		
	890-820		
Aromatic			
	1805-1780		
	1785-1755		
	1020-980		

Table 4.12. Ether Type Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
ETHERS			
Aliphatic			
O-CH_3	2830-2815		
C-O-C	1150-1060	1140	
O-$(CH_2)_4$	742-734		Diethyl ether
O-CH_3	1455		
Aromatic			
=C-O-C	1275-1200	1247	
C-O-C	1075-1020	1038	Anisol
Cyclic			
C-O-C	1140-1070		
Epoxides			
general	1260-1240	1261	1;2-Epoxybutane
trans compounds	890		
cis compounds	830	826	1;2-Epoxybutane
Tetrahydrofuran derivatives			
	1098-1075	1076	Tetrahydrofuran
	915-913	912	
Trioxans			
	1175	1172	Trioxan
	958	957	
Tetrahydropyran derivatives			
	1120-1080		
	1100-900		
	825-805		
Dioxan derivatives			
	1125	1122	Dioxan
KETALS, ACETALS			
R_2-C-$(O-C)_2$	1190-1158		
	1143-1124		
	1098-1063		

Table 4.13. Ketone and Aldehyde Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
KETONES			
Aliphatic			
	1725-1705	1727	Butanone
	1325-1215	1269	
	1200	1215	
Unsaturated			
C=C	1650-1620	1618	Methyl vinyl ketone
C=O	1685-1665	1684	
Aromatic			
Aryl, alkyl	1700-1680	1694	Acetophenone
Aryl, aryl	1670-1660		
Cyclic			
4- & 5-membered rings	1775-1740	1739	Cyclopentanone
6- & 7-membered rings	1725-1700	1703	Cycloheptanone
Diketones			
α-Diketones	1730-1710	1721	Diacyl ketone
β-Diketones	1640-1540		
γ-Diketones	1725-1705		
Halogen substituted			
α,α-Dihalogen substitution	1765-1745		
α-Dihalogen substitution	1745-1725		
ALDEHYDES			
General			
CH	2900-2700 2 band		
	2720-2700		
	975-780		
Aliphatic			
C=O	1740-1720	1735	Butyraldehyde
CH	1440-1325	1390	
Unsaturated			
C=O	1650-1620	1637	Crotonaldehyde
C=O α,β unsaturated	1690-1650		

Table 4.14. Carboxylic Acid Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
CARBOXYLIC ACIDS			
General			
OH	3200-2500 br		
CH	1440-1396		
	1320-1210		
OH dimer	950-900 br		
C=O halogen substitution	1740-1720		
C=O aliphatic	1720-1700	1718	Acetic acid
C=O unsaturated	1710-1690	1698	Crotonic acid
C=O aromatic	1700-1680	1695	Benzoic acid

Table 4.14. (Continued)

C=C	1660-1620	1655	Crotonic acid
Carboxylic Ions			
C=O	1610-1560		
C=O	1420-1300		

Table 4.15. Ester Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
ESTERS			
C=O unsaturated, aryl	1800-1770		
C=C unsaturated, aryl	1730-1710	1718	
C-O acrylates, fumarate	1300-1200	1282	Ethyl acetate
C-O	1190-1130		
C=O electronegatively substituted	1770-1745		
C=O α,γ keto	1755-1740		
C=O saturated	1750-1735	1744	Methyl acetate
C=O β keto	1660-1640		
C-O benzoates, phthalates	1310-1250	1277	Methyl benzoate
	1150-1100	1108	
C-O acetates	1250-1230	1246	Propyl acetate
	1060-1000	1047	
C-O phenolic acetates	1205		
C-O formate	1200-1180	1190	Propyl formate
LACTONES			
β-Lactones	1840-1800		
γ-Lactones	1780-1760	1776	Butyrolactone
δ-Lactones	1750-1730		
	1280-1150	1168	

Table 4.16. Anhydride Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
ANHYDRIDES			
Aliphatic			
C=O	1850-1800	1842	Acetic acid anhydride
C=O	1785-1760	1783	
C-O	1170-1050	1134	
Aromatic			
C=O	1880-1840	1866	Phthalic acid anhydride
C=O	1790-1770	1773	
C-O	1300-1200	1267	
Cyclic			
C=O	1870-1820	1818	Glutaric acid anhydride
C=O	1800-1750	1772	

Table 4.17. Amide Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
AMIDES			
Primary			
NH free	3500		
NH free	3400		
NH bridges	3350	3346	Butyramide
NH bridged	3190	3191	
C=O	1660-1640	1660	
	1430-1400	1430	
Secondary			
NH free *trans*	3460-3400		
NH free *cis*	3440-3420		
NH bridged *trans*	3320-3270	3280	N-Methylacetamide
NH bridged *cis*	3180-3140		
bridged *cis, trans*	3100-3070	3090	
C=O	1680-1630	1652	
NH	1570-1510	1564	
	720 br	725	
Tertiary			
C=O	1670-1630	1670	N,N-Dimethyl formamid

Table 4.18. Amino Acid Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
AMINO ACIDS			
NH	3130-3030 br		
	2760-2530		
	2140-2080		
C=O	1720-1680		
ionized form	1600-1560		
	1300		
C=O α-amino acids	1754-1720		
C=O β,γ-amino acids	1730-1700		
Amino acid HCl	3030-2500		
NH amino acid HCl's	1660-1590		
NH amino acid HCl's	1550-1490		

Table 4.19. Amine Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
AMINES			
General			
$N-CH_3$	2820-2730		
$N-CH_3$	1426		
C-N	1410		

Table 4.19. (Continued)

Aliphatic, primary			
NH free	3500-3200	3350	Ethylamine
	(2 bands)	3210	
NH	1650-1590	1630	
	1200-1150		
	1120-1030	1100	
Aliphatic, secondary			
NH free	3500-3200 1 band	3230	Dipropylamine
NH	1650-1550		
C-N	1200-1120	1126	
C-N	1150-1080	1090	
Aliphatic, tertiary			
C-N	1230-1130	1175	Ethyldimethylamine
C-N	1130-1030	1070	
Aromatic, primary			
	3510-3450	3460	Aniline
	3420-3380	3413	
	1630-1600	1621	
Aromatic, secondary			
Free	3450-3430		
Bridged	3400-3300	3400	N-Methylaniline

Table 4.20. Unsaturated Nitrogen Compouds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
UNSATURATED NITROGEN COMPOUNDS			
Imines			
NH	3400-3300		
C=N	1690-1640		
Oximes			
Liquid	3602-3590		
Solid	3250		
Solids	3115		
Aliphatic	1680-1665		
Aromatic	1650-1620		
	1300		
	900		

Table 4.21. Cyanide and Isocyanide Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
CYANIDES, ISOCYANIDES			
C≡N unconjugated	2265-2240	2256	Ethyl cyanide
C≡N conjugated or aromatic	2240-2220	2222	Benzyl cyanide
C≡N cyanide, thiocyanide complex	2200-2000		
N≡C alkyl isocyanide	2183-2150	2166	Methyl isocyanide
N≡C aryl isocyanide	2140-2080	2100	Phenyl isocyanide

Table 4.22. Cyclic Nitrogen Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
CYCLIC NITROGEN COMPOUNDS			
Pyridines, quinolines			
CH	3100-3000	3030	Pyridine
C=C, C=N	1615-1590	1590	
	1585-1550		
	1520-1465	1490	
	1440-1410		
	920-690	707	
Pyrimidines			
CH	3060-3010		
C=C, C=N	1580-1520		
Ring	1000-900		

Table 4.23. Unsaturated Nitrogen-Nitrogen Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
UNSATURATED NITROGEN-NITROGEN COMPOUNDS			
Azo compounds	1630-1575		
N=N azides	2160-2120	2130	Phenylazide
N=N azides	1340-1180	1297	

Table 4.24. Nitro Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
NITRO COMPOUNDS			
Aliphatic			
	1570-1500	1546	2-Nitrobutane
	1385-1365	1362	
	880	879	
Aromatic			
	1550-1510	1527	Nitrobenzene
	1370-1330	1351	
	849	853	

Table 4.25. Phosphorus Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
PHOSPHORUS COMPOUNDS			
O-H phosphoric acids	2700-2560 br		
P-H	2440-2350 sp		
P=O	1350-1250		
P=O	1250-1150		
P-O-C	1240-1190		
P-O-R	1190		
P-O-C	1170-1150		

Table 4.25. (Continued)

P-O-C	1050-990		
P-O-P	970-940		
P-F	885		
P=S	840-600		
O-P-H	865-840		
O-P-O	590-520		
O-P-O	460-440		
PHOSPHORUS-CARBON COMPOUNDS			
P-C aromatic	1450-1435		
P-C aliphatic	1320-1280	1298	Trimethylphosphine
P-C	750-650	707	
PO_4^{-3} aryl phosphates	1080-1040		
PO_4^{-3} alkyl phosphates	1180-1150		
PO_4^{-3} alkyl phosphates	1080		

Table 4.26. Deuterated Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
DEUTERATED COMPOUNDS			
O-D deuterated alcohols	2650-2400		
O-D deuterated carboxylic acids	675		

Table 4.27. Sulfur Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
SULFUR COMPOUNDS			
C=S	1400-1300	1357	Dithioacetic acid
S=S	1200-1050		
P=S	840-600		
SH mercaptans	2600-2550	2580	Ethyl mercaptan
C-S mercaptans	700-600	665	
C-S-C dialkyl sulfides	750-600	726	Methyl ethyl sulfide
	710-570	676	
	660-630	654	
Aliphatic sulphones	1410-1390	1407	Dimethylsulphone
	1350-1300	1316	
Sulphonic acids	1210-1150		
	1060-1030		
	650		

Table 4.28. Silicon Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
SILICON COMPOUNDS			
SiH alkylsilanes	2300-2100	2175	Dimethylsilane
$Si(CH_3)_2$	1265-1258	1262	

Table 4.28. (Continued)

	814-800		
	800		
$Si(CH_3)_3$	1260-1240	1259	Methoxytrimethylsilane
	850-830	844	
	760	763	
Si-C aromatic	1429		
	1130-1090		
Si-C	860-715		
Si-O siloxanes	1100-1000		
Si-O-C open-chain	1090-1020		
Si-O-Si open-chain	1097		
Si-O-Si cyclic	1080-1010		

Table 4.29. Halogen Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
HALOGEN COMPOUNDS			
Iodine Compounds			
	500		
Bromine Compounds			
	700-500		
Chlorine Compounds			
Monochloro	800-600		
	750-700		
Fully chlorinated compounds	780-710		
Fluorine Compounds			
	1400-1000		
	1100-1000		
Fully fluorinated compounds	745-730		

Table 4.30. Inorganic Compounds

Functional Group	Absorption Range (cm^{-1})	Example (cm^{-1})	Example Compound
INORGANIC COMPOUNDS			
Sulfates			
	1200-1140	1143	Potassium sulfate
	1130-1080	1117	
	680-610	617	
Nitrates			
	1380-1350	1370	Potassium nitrate
	840-815	825	
Nitrites			
	840-800		
	750		
Water of Crystallization			
	1630-1615		

Table 4.30. (Continued)

Halogen-Oxygen salts			
Chlorates	980-930	978	Potassium chlorate
	930-910	932	
Bromates	810-790	793	Potassium bromate
Iodates	785-730	756	Potassium iodate
Carbonates			
	1450-1410	1410	Calcium carbonate
	880-860	875	

4.4 Nuclear Magnetic Resonance Spectroscopy

4.4.1 Common NMR Solvents

Table 4.31. NMR Solvents

Compound	M.W.	$d^{20/4}$	m.p.[1]	b.p.[1]	δ^2_H(mult)[3]	δ^2_C(mult)[3]
Acetic Acid-d_4	64.078	1.12	17	118	11.53 (1) 2.03 (5)	178 (br) 20.0 (7)
Acetone-d_6	64.117	0.87	-94	57	2.04 (5)	206.0 (13) 29.8 (7)
Acetonitrile-d_3	44.071	0.84	-45	82	1.93 (5)	118.2 (br)
Benzene-d_6	84.152	0.95	5	80	7.15 (br)	128.0 (3)
Chloroform-d	120.384	1.50	-64	62	7.24 (1)	77.0 (3)
Cyclohexane-d_{12}	96.236	0.89	6	81	1.38 (br)	26.4 (5)
Deuterium Oxide	20.028	1.11	3.8	101.4	4.67 (TSP)	
1,2-Dichloroethane-d_4	102.985	1.25	-40	84	3.72 (br)	43.6 (5)
Diethyl-d_{10} Ether	84.185	0.82	-116	35	3.34 (m) 1.07 (m)	65.3 (5) 14.5 (7)
Dimethylformamide-d_7	80.138	1.04	-61	153	8.01 (br) 2.91 (5) 2.74 (5)	162.7 (3) 35.2 (7) 30.2 (7)
Dimethyl-d_6 Sulphoxide	84.170	1.18	18	189	2.49 (5)	39.5 (7)
p-Dioxane-d_8	96.156	1.13	122	101	3.53 (m)	66.5 (5)
Ethyl Alcohol-d_6	52.106	0.91	<-130	79	5.19 (1) 3.55 (br) 1.11 (m)	56.8 (5) 17.2 (7)

Table 4.31. (Continued)

Hexafluoroacetone Deuterate	198.067	1.71	21		5.26 (1)	122.5 (4) 92.9 (7)
HMPT-d_{18}	197.314	1.14	7	106	2.53 (2x5)	35.8 (7)
Methyl Alcohol-d_4	36.067	0.89	-98	65	4.78 (1)	49.0 (7)
Methylene Chloride-d_2	86.945	1.35	-95	40	5.32 (3)	53.8 (5)
Tetrahydrofuran-d_8	80.157	0.99	-109	66	3.58 (br) 1.73 (br)	67.4 (5) 25.3 (br)
Trifluoroacetic Acid-d	115.030	1.50	-15	72	11.50 (1)	164.2 (4) 116.6 (4)

1. Melting and boiling points (in ºC) are those of the corresponding light compounds. (except for D_2O) and are intended only to indicate the useful liquid range of the materials.
2. Chemicals shifts in ppm relative to TMS.
3. The multiplicity br indicates a broad peak without resolvable tine structure, while m indicates one with fine structure.
4. Note that chemical shifts can be dependent on solute, concentration and temperature.

4.4.2 Reference Standards for Proton NMR

Table 4.32. NMR Reference Standards

Compound (Abbrev.)	Formula	m.p. °C	b.p. °C	Hydrogen bands		
				Group[1]	δ	τ
Tetramethylsilane (TMS)[2]	$(CH_3)_4Si$		26.5	CH_3 (s)	0.00	10.00
Hexamethyl siloxane (HMDS)[3]	$[(CH_3)_3Si]_2O$	-59	100.4	CH_3 (s)	0.04	9.96
Sodium-3-trimethylsilyl-1-propane sulfonate (DSS)[4]	$(CH_3)_3Si$- CH_2-CH_2- CH_2-SO_3-Na	Solid Salt		CH_3 (s) 1-CH_2 (m) 2-CH_2 (m) 3-CH_2 (m)	0.00 0.6 1.8 2.9	10.00 9.4 8.2 7.1
Sodium 3-trimethylsilyl propionate-d_4 (TSP)[5]	$(CH_3)_3Si$- CD_2-CD_2- COO-Na	Solid Salt		CH_3 (s)	0.00	10.00

1. The functional group which produces the observed band. The multiplicity of the band is indicated in parenthesis; s = singlet; m = complex multiplet.
2. Primary reference standard for room temperature and below.
3. Can be used as reference up to 180º C.
4. Reference for water solutions. The CH_2 bands can interfere with weak sample bands.
5. Reference for water solutions.

4.4.3 NMR Proton Chemical Shift Chart

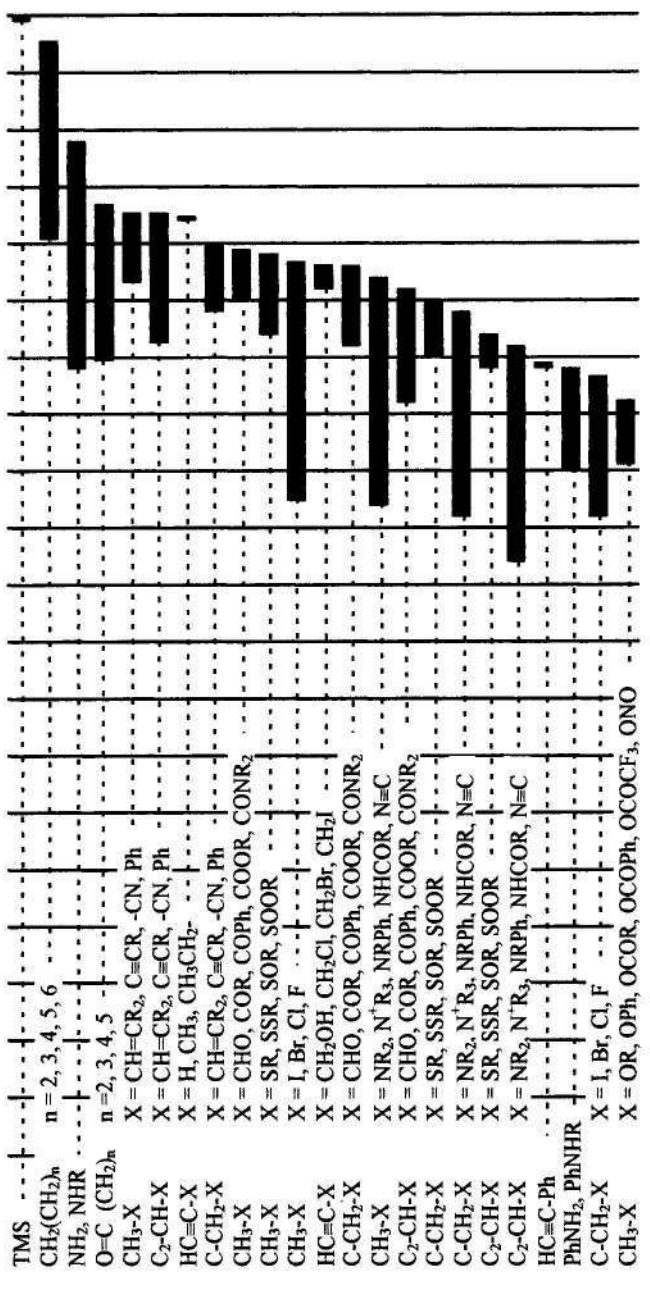


Table 4.33. Proton Chemical Shifts

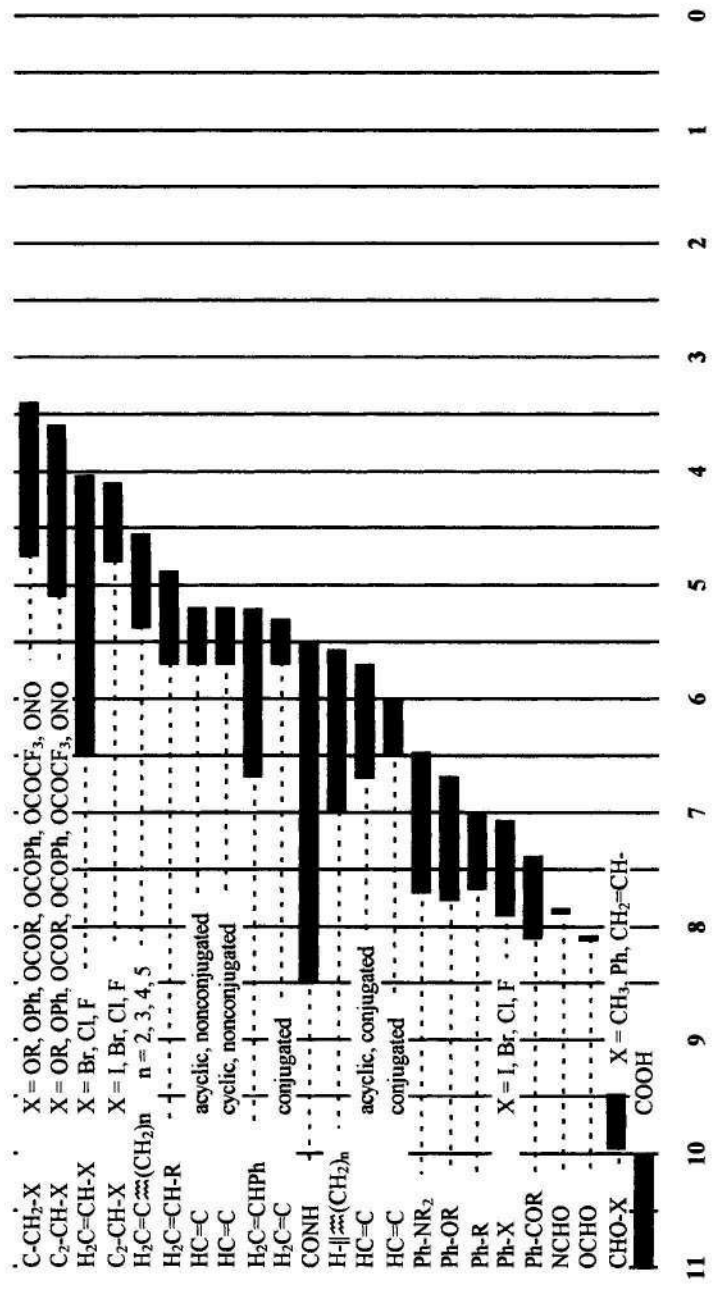


Table 4.33. (Continued)

4.4.4 NMR Chemical Shift Tables

The data in all of the tables are for the compound in dilute carbon tetrachloride or deuteriochloroform relative to internal TMS where such data were available. It is important to remember that solvent effects, especially in the case of aromatics, can cause significant variation in the observed chemical shifts. All chemical shifts listed are in ppm or δ.

Table 4.34. ^{1}H Chemical Shifts of Paraffinic Compounds with a Single Functional Groups

Group X	CH_3-X	C-CH_2-X	$(C)_2$-CH-X	CH_3-C-X	C-CH_2-C-X	$(C)_2$CH-C-X
-H	0.233	0.86	1.33	0.86	1.33	1.56
-CH=CR_2	1.73	2.00	1.73	1.55	1.35	1.00
-C≡CR	1.75	2.15	2.7	1.15	1.50	1.80
-C≡N	1.98	2.35	2.8	1.30	1.6	2.00
-Ph	2.34	2.60	2.87	1.18	1.6	1.8
-CHO	2.17	2.4	2.4	1.13	1.65	---
-COR	2.10	2.4	2.55	1.05	1.5	1.7
-COPh	2.5	2.9	3.4	1.18	1.6	2.0
-CO_2R	2.1	2.2	2.5	1.15	1.7	1.8
-$CONR_2$	2.05	2.23	2.4	1.1	1.6	1.8
-I	2.16	3.17	4.25	1.8	1.8	2.1
-Br	2.68	3.36	4.2	1.8	1.9	2.0
-Cl	3.05	3.44	4.1	1.5	1.8	2.0
-F	4.26	4.4	4.8	1.4	1.8	2.1
-OR	3.38	3.4	3.6	1.2	---	---
-OPh	3.82	3.95	4.6	1.3	1.5	1.7
-OCOR	3.65	4.1	5.0	1.25	1.6	1.8
-OCOPh	3.82	4.2	5.1	1.5	1.7	1.9
-$OCOCF_3$	3.95	4.3	---	1.4	1.6	---
-ONO	---	4.75	---	1.4	---	---
-NR_2	2.3	2.6	2.9	1.05	1.45	1.7
-N^+R_3	~3.2	~3.1	~3.6	1.4	1.7	2.0
-NRPh	~2.7	~3.1	~3.6	1.1	1.5	1.8
-NHCOR	2.8	3.3	3.8	1.1	1.5	1.9
-NO_2	4.30	4.4	4.6	1.6	2.05	2.5
-N≡C	2.85	---	4.8	1.6	---	---
-SR	2.09	2.5	3.0	1.25	1.6	1.9
-SSR	2.30	2.7	---	1.3	1.7	---
-SOR	2.5	3.0	2.8	1.35	1.7	---
-SO_2R	2.8	2.9	3.1	1.35	1.7	---

Table 4.35. ^{1}H Chemical Shifts of Paraffinic Compounds with Two Functional Groups

Y\X	CN	CF_3	Ph	C≡C	C=C	CH_3
CH_3	2.31	(1.84)	2.63	2.14	1.97	1.34
C=C	3.15	(2.69)	3.30	3.39	2.73	
C≡C	(3.37)	(2.81)	(3.52)	(3.11)		
Ph	3.68	3.50	3.92			
CF_3	(3.07)	(2.51)				
CN	4.13					

Y\X	COPh	$CONR_2$	COOR	COR
COR	(3.77)	3.52	3.32	3.62
COOR	(3.62)	(4.95)	4.22	
$CONR_2$	(3.66)	3.30		
COPh	(3.91)			

Y\X	OCOR	OPh	OR	OH
OH	(5.92)	(6.02)	(5.15)	(5.35)
OR	(5.72)	(5.82)	4.49	
OPh	(6.59)	(6.69)		
OCOR	(6.49)			

Y\X	I	Br	Cl
Cl	4.99	5.16	5.28
Br	(4.38)	4.94	
I	3.89		

Y\X	NHCOR	N_3	NR_2
NR_2	(4.07)	(3.77)	3.10
N_3	(4.47)	(4.17)	
NHCOR	(4.77)		

Values in parentheses were calculated by the emperical method of Shoolery. All values refer to methylene (CH_2) protons in $X\text{-}CH_2\text{-}Y$.

Table 4.36. ^{1}H Chemical Shifts of Olefinic Compounds

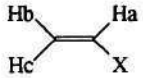
Compound	X=	a	b	c
$H_2C{=}CH_2$		5.33		
	R	5.70	4.88	4.96
	F	6.17	4.03	4.37
	Cl	6.30	5.44	5.52
	Br	6.49	5.88	6.03
	C_6H_5	6.69	5.21	5.71
	CCl_3	6.41	5.30	5.78
	CN	5.53	6.05	5.78
	CH_2OH	6.00	5.13	5.25
	OCH_3	6.43	3.90	4.04

Table 4.36. (Continued)

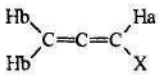
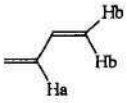
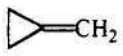
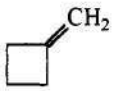
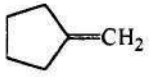
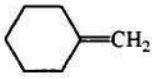
$H_2C{=}C{=}CH_2$		4.55		
	Cl Br I	5.76 5.85 5.62	5.05 4.82 4.46	
		5.20	5.11	
		5.38		
		4.70		
		4.82		
		4.55		
CH_3-**CHO**		9.72		
Ph-**CHO**		9.96		
CH_2=CH-**CHO**		9.48		
$(CH_3)_2$N-**CHO**		7.84		
CH_3O-**CHO**		8.08		

Table 4.37. ^{1}H Chemical Shifts of Acetylenic Compounds

Compound	δ	Compound	δ
H-C≡C-**H**	1.80	OHC-C≡C-**H**	1.89
CH_3-C≡C-**H**	1.80	$HOCH_2$-C≡C-**H**	2.33
CH_3CH_2-C≡C-**H**	1.76	Cl-CH_2-C≡C-**H**	2.40
Ph-C≡C-**H**	3.05	Br-CH_2-C≡C-**H**	2.33
CH_2=CH-C≡C-**H**	2.92	I-CH_2-C≡C-**H**	2.19
C_2H_5-C≡C-C≡C-**H**	1.95	CH_3O-C≡C-**H**	1.33
$CH_3(C{\equiv}C)_2$C≡C-**H**	1.87	CH_2=CH-O-C≡C-**H**	1.89

Table 4.38. ^{1}H Chemical Shifts of Cycloparaffinic Compounds

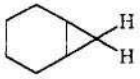
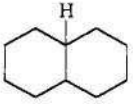
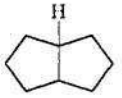
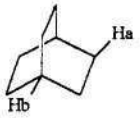
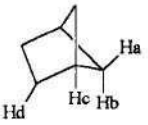
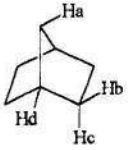
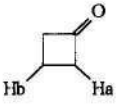
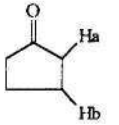
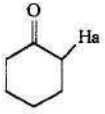
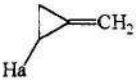
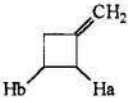
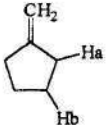
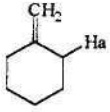
Compound	δ	Compound	δ	Compound	δ
Cyclopropane	0.22	Cylcobutane	1.96	Cyclopentane	1.51
Cyclohexane	1.44	Cycloheptane	1.54	Cyclooctane	1.54
Adamantane	1.78				
	0.02		~1.4		2.37
	a 1.51 b ~2.1		a 1.56 b 0.87 c 2.49 d 1.58		a 1.21 b 1.49 c 1.18 d 2.20
	1.65		a 3.03 b 1.96		a 2.06 b 2.02
	2.25		0.99		a 2.70 b 1.92
	a 2.70 b 1.92		1.5		

Table 4.39. ^{1}H Chemical Shifts Of Cycloolefinic Compounds

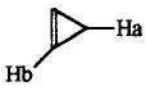
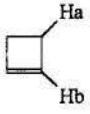
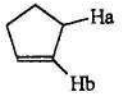
Compound	δ	Compound	δ	Compound	δ
	a 0.92 b 7.01		a 2.57 b 5.97		a 2.28 b 5.60

Table 4.39. (Continued)

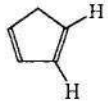
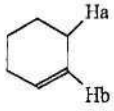
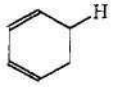
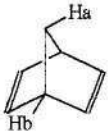
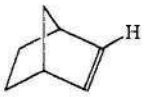
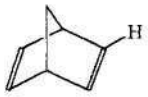
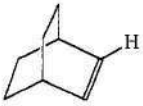
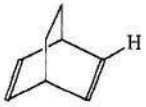
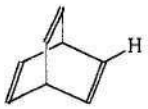
 6.42	 a 1.96 b 5.57	 2.15
 a 1.95 b 3.53	 5.95	 6.66
 6.25	 6.27	 6.70

Table 4.40. ^{1}H Chemical Shifts Of Monosubstituted Benzenes

Substituent	Ortho	Meta	Para
H	7.27	7.27	7.27
CH_3	7.07	7.07	7.07
CH_2CH_3	7.13	7.13	7.13
CH_2OH	7.28	7.28	7.28
CH_2Cl	7.32	7.32	7.32
$CHCl_2$	7.42	7.42	7.42
CCl_3	7.91	7.40	7.37
$CH=CH_2$	7.5	7.5	7.5
CHO	7.83	7.49	7.56
$COCH_3$	7.89	7.41	7.56
CO_2H	8.12	7.43	7.51
CO_2CH_3	7.98	7.38	7.48
COCl	8.11	7.49	7.63
COBr	8.07	7.48	7.64
$CONH_2$	7.8	7.5	7.5
CN	7.63	7.45	7.55
F	6.99	7.24	7.08
Cl	7.30	7.25	7.18
Br	7.45	7.19	7.23
I	7.67	7.06	7.27
NH_2	6.52	7.02	6.62
$NHCH_3$	6.47	7.05	6.59
$N(CH3)_2$	6.61	7.09	6.60
$NHCOCH_3$	7.7	7.1	7.0

Table 4.40. (Continued)

NH_3^+	7.7	7.5	7.5
NO	7.81	7.55	7.61
NO_2	8.22	7.53	7.65
OH	6.68	7.15	6.82
OCH_3	7.77	7.15	7.37
$OCOCH_3$	6.79	7.18	6.83
SCH_3	7.4	7.2	7.1
SO_2Cl	8.04	7.62	7.72
SO_3CH_3	7.87	7.53	7.60

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Table 4.41. ^{1}H Chemical Shifts Of Heteroaromatic Compounds

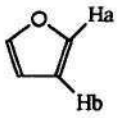
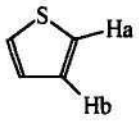
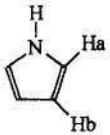
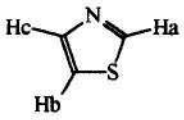
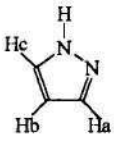
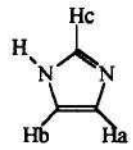
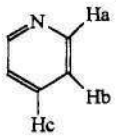
Compound	δ	Compound	δ
	a 7.38 b 6.30		a 7.19 b 7.04
	8.19		8.58
	a 6.62 b 6.05		a 8.88 b 7.41 c 7.98
	a 7.55 b 6.25 c 7.55		a 7.14 b 7.14 c 7.70
	a 8.50 b 7.06 c 7.46		a 6.57 b 7.26 c 6.15 d 7.13

Table 4.41. (Continued)

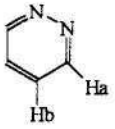
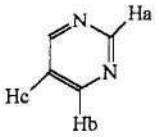
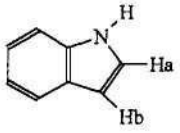
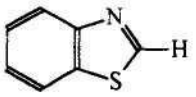
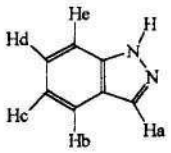
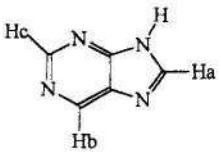
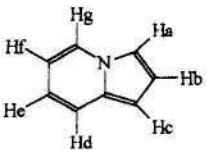
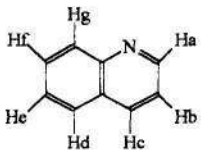
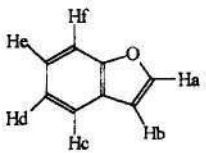
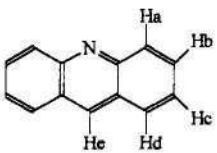
	a 9.17 b 7.68		a 9.15 b 8.60 c 7.09
	8.5		9.18
	a 6.54 b 6.34		8.95
	a 8.03 b 7.77 c 7.12 d 7.34 e 7.58		a 8.63 b 9.16 c 8.95
	a 7.14 b 6.64 c 6.28 d 7.25 e 6.50 f 6.35 g 7.76		a 8.81 b 7.26 c 8.00 d 7.68 e 7.43 f 7.61 g 8.05
	a 7.52 b 6.66 c 7.49 d 7.13 e 7.19 f 7.42		a 8.20 b 7.69 c 7.39 d 7.80 e 8.53

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Table 4.42. ^{1}H Chemical Shifts Of Heterocyclic Compounds

Compound	δ	Compound	δ	Compound	δ
	2.54		1.48		2.27

Table 4.42. (Continued)

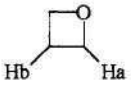
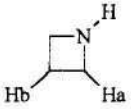
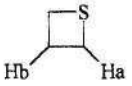
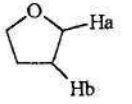
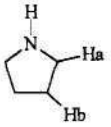
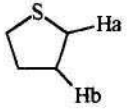
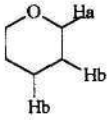
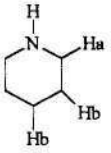
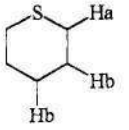
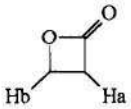
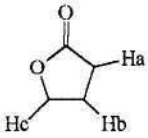
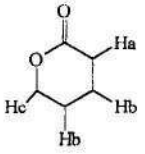
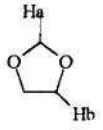
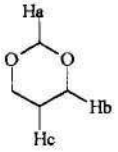
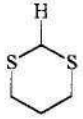
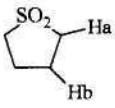
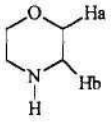
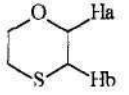
 a 4.73 b 2.72	 a 3.54 b 2.23	 a 2.82 b 1.93
 a 3.63 b 1.79	 a 2.74 b 1.62	 a 2.82 b 1.93
 a 3.56 b 1.58	 a 2.69 b 1.49	 a 2.57 b 1.60
 a 3.48 b 4.22	 a 2.31 b 2.08 c 4.28	 a 2.27 b 1.62 c 4.06
 a 4.77 b 3.77	 a 4.82 b 3.80 c 1.68	 3.59
 5.00	 3.69	 4.18
 a 2.92 b 2.16	 a 3.57 b 2.83	 a 3.88 b 2.57

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Table 4.43. ^1H Chemical Shifts of Hydrogen Bonded To Oxygen, Nitrogen, Sulfur

Compound	δ	Compound	δ
ROH (monomeric)[a]	0.5	Oximes	7-11
ROH (hydrogen bonded)	0.5-5.0	RNH_2	1.1-1.8
ArOH (monomeric)[a]	4.5	R_2NH	1.2-2.1
ArOH (hydrogen bonded)	4.5-9	$ArNH_2$	3.3-4.0
Enols (intramolecular bonded)	15-19	ArNHR	3.1-3.8
Carboxylic acids	10-13	$RCONH_2$, $ArCONH_2$	5-6.5
Sulfonic acids	11-12	RCONHR, ArCONHR	6-8.2
RSH	1-2	RCONHAr, ArCONHAr	7.8-9.4
ArSH	3-4	R_3N^+H	7.1-7.7

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4.5 Mass Spectroscopy

4.5.1 Common Molecular Ions Table

Table 4.44. Common Elemental Compositions of Molecular Ions[1]

m/z	Composition
16	CH_4
17	NH_3
18	H_20
26	C_2H_2
27	CHN
28	C_2H_4, CO, N_2
30	C_2H_6, CH_2O, NO
31	CH_5N
32	CH_4O, N_2H_4, SiH_4, O_2
34	CH_3F, PH_3, H_2S
36	HCl
40	C_3H_4
41	C_2H_3N
42	C_3H_6, C_2H_2O, CH_2N_2
43	C_2H_5N, N_3H
44	C_2H_4O, C_3H_8, C_2HF, CO_2, N_2O
45	C_2H_7N, CH_3NO
46	C_2H_6O, C_2H_3F, CH_6SI, CH_2O_2, NO_2
48	C_2H_5F, CH_4S, CH_5P
50	C_4H_2, CH_3Cl
52	C_4H_4, CH_2F_2
53	C_3H_3N, HF_2N
54	C_4H_6, F_2O
55	C_3H_5N
56	C_4H_8, C_3H_4O, $C_2H_4N_2$
57	C_3H_7N, C_2H_3NO

Table 4.44. (Continued)

58	C_3H_6O, C_4H_{10}, $C_2H_2O_2$, $C_2H_6N_2$
59	C_3H_9N, C_2H_5NO, CH_5N_3
60	C_3H_8O, C_3H_5F, C_2H_8N2, $C_2H_4O_2$, C_2H_8Si, C_2H_4S, C_2HCl, CH_4N_2O, COS
61	C_2H_7NO, CH_3NO_2, $CClN$
62	C_3H_7F, C_2H_7P, $C_2H_6O_2$, C_2H_6S, C_2H_3Cl
64	$C_2H_2F_2$, C_2H_5FO, C_2H_5CL, SO_2
66	C_5H_6, $C_2H_4F_2$, CF_2O, F_2N_2
67	C_4H_5N, CH_3F_2N, ClO_2
68	C_5H_8, C_4H_4O, $C_3H_4N_2$, C_3O_2, CH_2ClF
69	C_4H_7N, C_3H_3NO, $C_2H_3N_3$
70	C_5H_{10}, C_4H_6O, $C_3H_6N_2$, CH_2N_4, CHF_3
71	C_4H_9N, C_3H_5NO, F_3N
72	C_4H_8O, C_5H_{12}, $C_3H_4O_2$, C_4H_5F
73	$C_4H_{11}N$, C_3H_7NO, C_2H_3NS, $C_2H_7N_3$
74	$C_4H_{10}O$, $C_3H_6O_2$, $C_3H_{10}N_2$, C_3H_6S, $C_2H_6N_2O$, $C_3H_{10}Si$, C_3H_3Cl, CH_6N_4, $C_2H_6N_2O$, $C_2H_2O_3$,
75	C_3H_9NO, $C_2H_5NO_2$, C_2H_2ClN
76	$C_3H_8O_2$, C_3H_8S, C_3H_5Cl, C_4H_9F, C_4N_2, C_3H_9P, C_3H_5FO, $C_2H_4O_3$, C_2H_4OS, CH_8Si_2, CH_4N_2S, CS_2
77	CH_3NO_3
78	C_6H_6, C_3H_7Cl, C_4HSN_2, C_2H_6OS, C_2H_3ClO, $C_2H_3FO_2$, CF_2N_2, $CH_6N_2O_2$
79	C_5H_5N
80	C_6H_8, $C_4H_4N_2$, $C_3H_6F_2$, C_2H_5ClO, C_2H_2ClF, CH_4O_2S, HBr
81	C_5H_7N, $C_3H_3N_3$, $C_2H_5F_2N$
82	C_6H_{10}, $C_4H_6N_2$, C_5H_6O, C_2H_4ClF, $C_2H_2N_4$, C_2HF_3, $CClFO$
83	C_5H_9N, $C_3H_5N_3$, C_4H_5NO
84	C_6H_{12}, C_5H_8O, $C_4H_8N_2$, $C_4H_4O_2$, $C_2H_4N_4$, C_4H_4S, $C_2H_3F_3$, CH_2Cl_2
85	$C_5H_{11}N$, C_4H_7NO, C_3H_3NS, CH_3N_5
86	$C_5H_{10}O$, $C_4H_6O_2$, C_6H_{14}, $C_4H_{10}N_2$, C_4H_6S, C_4H_3Cl, $C_3H_6N_2O$, $C_2H_2N_2S$, $CHClF_2$, HF_2O, Cl_2O, F_2OS
87	$C_5H_{13}N$, C_4H_9NO, $C_3H_9N_3$, C_3H_5NS, C_3H_2ClN, ClF_2N, F_3NO
88	$C_5H_{12}O$, $C_4H_8O_2$, $C_4H_{12}N_2$, C_4H_8S, $C_3H_8N_2O$, $C_3H_4O_3$, $C_4H_{12}Si$, C_4H_5Cl, CF_4
89	$C_4H_{11}NO$, $C_3H_7NO_2$, C_3H_4ClN
90	$C_4H_{10}O_2$, $C_4H_{10}S$, C_4H_7Cl, $C_3H_6O_3$, $C_3H_{10}OSi$, C_3H_6OS, C_3H_3ClO, $C_2H_6N_2O_2$, $C_2H_6N_2S$, $C_2H_2O_4$, $C_4H_{11}P$
91	$C_2H_5NO_3$, CH_5N_3S, C_3H_6ClN
92	C_7H_8, C_4H_9Cl, C_3H_5ClO, $C_2H_4O_2S$, $C_3H_8O_3$, C_3H_9FSi, $C_5H_4N_2$, C_6H_4O
93	C_6H_7N, C_5H_3NO, $C_4H_3N_3$
94	$C_5H_6N_2$, C_7H_{10}, C_6H_6O, C_3H_7ClO, $C_2H_2S_2$, $C_2H_6O_2SC_3HF_3$, $C_2H_3ClO_2$ C_2Cl_2, CH_3Br
95	C_5H_5NO, C_6H_9N, $C_4H_5N_3$, C_2F_3N
96	C_7H_{12}, C_6H_8O, $C_5H_8N_2$, $C_5H_4O_2$, $C_4H_4N_2O$, $C_2H_2Cl_2$, $C_3H_3F_3$, $C_2H_6F_2Si$
97	C_5H_7NO, $C_6H_{11}N$
98	C_7H_{14}, $C_6H_{10}O$, $C_5H_6O_2$, $C_4H_6O_2$, $C_4H_6N_2O$, $C_3H_6N_4$, $C_5H_{16}N_2$, C_5H_6S C_4H_2,O_3, $C_2H_4Cl_2$, C_2HClF_2, CCl_2O
99	$C_6H_{13}N$, C_5H_9NO, C_4H_5NS, $C_4H_5NO_2$, CH_3F_2NS

Table 4.44. (Continued)

100	$C_6H_{12}O$, $C_5H_8O_2$, C_7H_{16}, $C_4H_4O_3$, $C_3H_4N_2S$, $C_5H_{12}N_2$, C_6H_9F, $C_5H_{12}Si$, C_4H_4OS, $C_3H_4N_2O_2$, $C_2H_3F_3O$, C_2F_4
101	$C_6H_{15}N$, $C_5H_{11}NO$, $C_4H_7NO_2$, C_4H_7NS, $C_2H_3N_3S$
102	$C_6H_{14}O$, $C_5H_{10}O_2$, $C_5H_{10}S$, $C_4H_{10}N_2O$, $C_4H_6O_3$, $C_2H_2F_4$, $C_3H_6N_2S$, C_8H_6, $CHCl_2F$, CHF_3S, HF_2PS, Cl_2S
103	$C_4H_9NO_2$, C_7H_5N, $C_5H_{13}NO$, $C_4H_{13}N_3$, C_4H_6ClN, $C_2H_2ClN_3$
104	$C_5H_{12}O_2$, $C_5H_{12}S$, C_5H_9Cl, $C_4H_8O_3$, $C_4H_8O_3$, C_4H_8OS, C_8H_8, $C_6H_{13}F$, $C_6H_4N_2$, $C_4H_{12}N_2O$, $C_4H_{12}OSi$, C_4H_5ClO, $C_3H_8N_2S$, $CClF_3$, SiF_4
105	C_7H_7N, $C_3H_7NO_3$, $C_4H_{11}NO_2$, C_4H_8ClN, $CBrN$
106	C_8H_{10}, $C_5H_{11}Cl$, $C_6H_6N_2$, C_7H_6O, $C_4H_{10}O_3$, C_4H_7ClO, $C_4H_{10}OS$, $C_3H_6O_2S$, C_2H_3Br
107	C_7H_9N, C_6H_5NO. $C_2H_5NO_4$
108	$C_6H_8N_2$, C_8H_{12}, C_7H_8O, C_4H_9ClO, C_3H_9ClSi, $C_3H_3ClO_2$, $C_6H_4O_2$, $C_3H_8S_2$, C_2H_5Br, $C_2H_4O_3S$, SF_4
109	C_6H_7NO, $C_7H_{11}N$, $C_2H_4ClNO_2$
110	C_8H_{14}, $C_7H_{10}O$, $C_5H_6N_2O$, $C_3H_4Cl_2$, C_7H_7F, $C_6H_6O_2$, $C_4H_6N_4$, $C_2H_6O_3S$, $C_2H_7O_3P$, $C_3H_7ClO_2$, $C_6H_{10}N_2$
111	$C_7H_{13}N$, C_6H_9NO, $C_5H_5NO_2$, $C_4H_5N_3O$, C_2ClF_2N, C_6H_6FN, $C_5H_9N_3$, C_5H_5NS
112	C_8H_{16}, $C_7H_{12}O$, $C_6H_8O_2$, $C_6H_{12}N_2$, $C_6H_{12}N_2$, C_6H_8S, $C_5H_8N_2O$, $C_5H_4O_3$, $C_4H_4N_2O_2$, $C_3H_6Cl_2$, C_6H_5FO, C_6H_5Cl, C_5H_4OS, C_3F_4, $C_3H_3F_3O$, CH_2BrF
113	$C_7H_{15}N$, $C_6H_{11}NO$, $C_5H_7NO_2$, C_5H_7NS, C_5H_4ClN, $C_3H_3NO_2$, $C_2H_6F_2NP$
114	$C_7H_{14}O$, $C_6H_{10}O_2$, C_8H_{18}, $C_6H_{14}N_2$, $C_4H_6N_2O_2$, $C_5H_6N_2O_2$, C_5H_6OS, $C_6H_4F_2$, $C_5H_2O_3$, C_6H_7Cl, $C_4H_6N_2S$, $C_2H_4Cl_2O$, C_2HCl_2F, C_2HClF_2O, $C_2HF_3O_2$
115	$C_6H_{13}NO$, $C_7H_{17}N$, $C_5H_9NO_2$, C_5H_9NS, C_4H_5NOS, $C_3H_5N_3S$, $C_5H_{13}N_3$
116	$C_6H_{12}O_2$, $C_7H_{16}O$, $C_6H_{12}S$, C_9H_8, $C_6H_{16}N_2$, $C_6H_{16}Si$, C_6H_9Cl, $C_5H_{12}N_2O$, $C_5H_8O_3$, $C_4H_8N_2O_2$,$C_4H_4O_4$, $C_4H_8N_2S$, $C_4H_4S_2$, $C_2H_3Cl_2F$, C_2ClF
117	C_8H_7N, $C_6H_{15}NO$, $C_5H_{11}NO_2$, C_5H_6ClN, $C_4H_7NO_3$, C_3H_4ClN
118	$C_6H_{14}O_2$, $C_6H_{14}S$, $C_5H_{10}O_3$, C_9H_{10}, $C_7H_{16}N_2$, $C_5H_{10}OS$, $C_6H_{15}P$, $C_7H_{15}F$, $C_6H_{11}Cl$, $C_5H_{14}OSi$, $C_4H_{10}N_2O_2$, $C_4H_6O_4$, C_4H_3ClS, $C_4H_{10}N_2S$, $C_4H_{14}Si_2$, C_3H_3Br, $C_2H_2ClF_3$, $CHCl_3$
119	C_7H_5NO, $C_6H_4N_3$, C_8H_9N, $C_4H_9NO_3$, C_4H_9NOS
120	C_9H_{12}, C_8H_8O, $C_4H_8O_2S$, $C_4H_8S_2$, $C_7H_8S_2$, $C_7H_8N_2$, $C_6H_{13}Cl$, $C_5H_{12}O_3$, $C_6H_4N_2O$, $C_5H_4N_4$, $C_4H_8O_4$, C_5H_9OCl, $C_4H_{12}O_2Si$, C_3H_5Br, CCl_2F_2
121	$C_8H_{11}N$, C_7H_7NO, $C_6H_7N_3$, $C_4H_3N_5$, C_7H_3FN
122	$C_8H_{10}O$, $C_7H_{10}N_2$, $C_7H_6O_2$, $C_4H_7ClO_2$, $C_4H_{10}S_2$, C_9H_{14}, C_3H_7Br, C_8H_7F, $C_6H_6N_2O$, $C_4H_{10}O_2S$, $C_4H_4Cl_2$, $C_3H_6O_3S$, $C_2H_6N_2S_2$, C_2H_3BrO
123	C_7H_9NO, $C_6H_5NO_2$, $C_8H_{13}N$, $C_6H_9N_3$, $C_4H_4F_3N$, $C_3H_9NO_2S$
124	$C_3H_8O_3S$, C_8H_9F, $C_7H_{12}N_2$, C_7H_5FO, $C_5H_4N_2O_2$, $C_4H_6F_2O_2$, $C_3H_5ClO_3$, C_2H_5BrO, $C_2H_4S_3$
125	$C_8H_{15}N$, $C_6H_{11}N_3$, C_6H_7NS, $C_7H_{11}NO$, $C_6H_7NO_2$, $C_2H_8NO_3P$, $C_2H_4ClNO_3$
126	C_9H_{18}, $C_8H_{14}O$, $C_4H_8Cl_2$, $C_7H_{10}O_2$, $C_5H_6N_2O_2$, C_7H_7Cl, $C_6H_{10}N_2O$, $C_6H_6O_3$, $C_7H_{10}S$, $C_3H_4Cl_2$, $C_2H_6S_3$, $C_7H_{14}N_2$, C_7H_7FO, C_6H_6OS, $C_4H_6N_4O$, $C_4H_5F_3O$, $C_3H_2N_6$, C_2ClO_2
127	$C_7H_{13}NO$, $C_8H_{17}N$, C_6H_2ClN, $C_5H_9N_3O$, $C_5H_5NO_3$, $C_6H_9NO_2$, $C_4H_5N_3S$, C_2Cl_2FN

Table 4.44. (Continued)

128	$C_8H_{16}O$, C_9H_{20}, $C_7H_{12}O_2$, $C_7H_{12}O_2$, $C_7H_{12}S$, $C_8H_4N_2$, $C_6H_8O_3$, C_6H_6OS, C_6H_5ClO, $C_4H_4N_2OS$, $C_3H_6Cl_2O$, $C_{10}H_8$, $C_2H_6Cl_2Si$, $C_2H_2Cl_2O_2$, CH_2BrCl, $C_2H_5ClO_2S$, $C_8H_{13}F$, HI
129	$C_8H_{19}N$, $C_7H_{15}NO$, $C_6H_{11}NO_2$, C_9H_7N, $C_7H_3N_3$, $C_6H_{15}N_3$, $C_5H_7NO_3$, C_5H_7NOS, $C_4H_7N_3S$, $C_4H_4ClN_3$, $C_4H_3NO_2S$
130	$C_7H_{14}O_2$, $C_8H_{18}O$, $C_6H_{10}O_3$, $C_6H_6N_2$, $C_{10}H_{10}$, C_9H_6O, $C_7H_{14}S$, $C_6H_{14}N_2O$, C_6H_4ClF, $C_5H_6O_4$, $C_5H_6S_2$, $C_3H_5Cl_2F$, $C_5H_{10}N_2O_2$, $C_3H_6N_4S$, $C_3H_2ClF_3$, $C_3H_2N_2O_2S$, C_2HCl_3, $CHBrF_2$
131	C_9H_9N, $C_7H_{17}NO$, $C_5H_9NO_3$, $C_7H_5N_3$, $C_6H_{17}N_3$, $C_6H_{13}NO_2$, $C_4H_9N_3S$, CF_3NOS
132	$C_7H_{16}O_2$, $C_6H_{12}O_3$, $C_{10}H_{12}$, C_9H_8O, $C_7H_{16}S$, $C_8H_8N_2$, $C_6H_{16}OSi$, $C_5H_8O_4$, $C_6H_{12}OS$, C_6H_9ClO, $C_5H_{12}N_2O_2$, $C_5H_{12}N_2S$, $C_5H_8O_2S$, $C_5H_5ClO_2$, $C_4H_4OS_2$, $C_3H_{12}Si_3$, $C_3H_4N_2S_2$, $C_2H_3Cl_3$, $C_2Cl_2F_2$, $C_2F_4O_2$
133	$C_9H_{11}N$, C_8H_7NO, $C_7H_7N_3$, $C_5H_{11}NO_3$, $C_4H_7NO_2S$, C_3H_4BrN, $C_2H_3ClF_3N$
134	$C_9H_{10}O$, $C_{10}H_{14}$, $C_6H_{14}O_3$, $C_6H_6N_4$, $C_5H_{10}O_2S$, $C_8H_6O_2$, $C_8H_6O_2$, $C_8H_{10}N_2$, C_8H_6S, $C_7H_{15}Cl$, $C_7H_6N_2O$, $C_6H_{14}OS$, $C_6H_{11}ClO$, $C_5H_{11}ClSi$, $C_5H_{10}S_2$, $C_5H_7ClO_2$, $C_3H_3F_5$, $C_3Cl_2N_2$, $C_2H_2Cl_2F_2$
135	$C_9H_{13}N$, C_8H_9NO, C_7H_5NS, $C_5H_5N_5$, $C_7H_5NO_2$, $C_6H_5N_3O$, $C_4H_9NO_2S$, C_3H_6BrN, $C_3F_3N_3$
136	$C_9H_{12}O$, $C_{10}H_{16}$, $C_8H_8O_2$, C_4H_9Br, $C_8H_{12}N_2$, $C_8H_{12}Si$, C_8H_8S, C_8H_5Cl, $C_7H_8N_2O$, $C_7H_4O_3$, $C_5H_{12}S_2$, $C_6H_4N_2O_2$, $C_6H_4N_2O_2$, $C_6H_4N_2S$, $C_5H_{12}O_4$, $C_5H_{12}OS$, $C_5H_9ClO_2$, $C_5H_4N_4O$, C_2HClF_4, CCl_3F
137	$C_8H_{11}NO$, $C_9H_{15}N$, $C_7H_7NO_2$, C_7H_7NS, C_7H_4ClN, $C_6H_7N_3O$, $C_5H_6F_3N$, $C_5H_3N_3S$, $C_3H_7NO_5$
138	$C_{10}H_{18}$, $C_9H_{14}O$, $C_8H_{10}O_2$, $C_8H_{10}S$, $C_7H_6O_3$, $C_6H_6N_2O_2$, C_8H_7Cl, $C_7H_{10}N_2O$, C_7H_6OS, $C_6H_{10}N_4$, $C_5H_6N_4O$, $C_4H_{11}O_3P$, $C_4H_{10}O_3S$, C_3H_7BrO, $C_3H_6S_3$, $C_2H_3BrO_2$, C_2F_6
139	C_7H_9NS, $C_9H_{17}N$, $C_7H_{13}N_3$, $C_7H_9NO_2$, $C_6H_5NO_3$, $C_5H_5N_3O_2$, C_6H_5NOS
140	$C_9H_{16}O$, $C_{10}H_{20}$, C_8H_9Cl, $C_8H_{12}O_2$, $C_8H_{12}S$, $C_7H_8O_3$, $C_5H_{10}Cl_2$, C_7H_8OS, C_8H_9FO, $C_8H_{16}N_2$, $C_8H_6F_2$, C_7H_5ClO, $C_6H_8N_2O_2$, $C_6H_8N_2S$, $C_6H_4O_4$, $C_6H_4S_2$, $C_4H_6Cl_2O$, C_2H_2BrCl
141	$C_8H_{15}NO$, $C_7H_{11}NO_2$, $C_6H_{11}N_3O$, $C_6H_7NO_3$, $C_9H_{19}N$, $C_7H_{15}N_3$, $C_5H_7N_3S$, $C_4H_6F_3NO$, $C_4H_3F_4N$
142	$C_8H_{14}O_2$, $C_9H_{18}O$, $C_{10}H_{22}$, $C_6H_6O_4$, $C_8H_{14}S$, $C_3H_4Cl_2O_2$, C_7H_7ClO, $C_{11}H_{10}$, $C_9H_{15}F$, $C_8H_{18}N_2$, $C_7H_{14}N_2O$, $C_7H_{10}O_3$, $C_6H_{10}N_2O_2$, $C_6H_6O_2S$, $C_5H_6N_2OS$, $C_4H_8Cl_2O$, $C_4H_5ClF_2O$, C_2H_4BrCl, C_2HBrF_2, CH_3I
143	$C_{10}H_9N$, $C_8H_{17}NO$, $C_7H_{13}NO_2$, $C_9H_{21}N$, $C_7H_{10}ClN$, $C_6H_{13}N_3O$, $C_6H_9NO_3$, C_4H_9NOS, $C_5H_9N_3S$, C_2Cl_3N
144	$C_8H_{16}O_2$, $C_9H_{20}O$, $C_9H_8N_2$, $C_7H_{12}O_3$, $C_6H_8O_4$, $C_{10}H_8O$, $C_{11}H_{12}$, $C_8H_{16}S$, $C_8H_{13}Cl$, $C_7H_{16}N_2O$, $C_7H_{12}OS$, $C_6H_9ClN_2$, $C_5H_8N_2O_3$, $C_3H_3Cl_3$
145	$C_{10}H_{11}N$, C_9H_7NO, $C_8H_7N_3$, $C_7H_{15}NO_2$, $C_6H_{11}NO_3$, $C_5H_{11}N_3S$, $C_3H_3N_3O_2S$
146	$C_8H_{18}O_2$, $C_7H_{14}O_3$, $C_8H_{18}S$, $C_6H_{10}O_4$, $C_6H_{10}O_2S$, $C_{11}H_{14}$, $C_{10}H_{10}O$, $C_9H_{10}N_2$, $C_{10}H_7F$, $C_8H_6N_2O$, $C_7H_{18}OSi$, $C_7H_{14}OS$, $C_7H_6N_4$, $C_6H_{14}N_2O_2$, $C_6H_4Cl_2$, $C_5H_6OS_2$, $C_3H_5Cl_3$, $C_3H_3BrN_2$, C_2HCl_3O, $CHBrClF$
147	$C_{10}H_{13}N$, C_9H_9NO, $C_8H_9N_3$, $C_8H_5NO_2$, $C_7H_5N_3O$, $C_6H_{13}NO_3$, $C_5H_9NO_4$, $C_2H_2BrN_3$

Table 4.44. (Continued)

148	$C_{11}H_{16}$, $C_{10}H_{12}O$, $C_9H_8O_2$, $C_7H_8N_4$, $C_9H_{12}N_2$, $C_6H_{12}O_2S$, $C_8H_{17}Cl$, $C_8H_8N_2O$, $C_8H_4O_3$, C_9H_8S, $C_7H_{16}O_3$, $C_7H_{16}OS$, $C_7H_4N_2O_2$, $C_6H_{12}O_4$, $C_6H_4N_4O$, $C_5H_8O_3S$, C_3HF_5O, $C_2H_3Cl_3O$, C_2Cl_3F, $CBrF_3$
149	$C_{10}H_{15}N$, $C_9H_{11}NO$, $C_7H_7N_3O$, $C_8H_{11}N_3$, $C_8H_7NO_2$
150	$C_{10}H_{14}O$, $C_9H_{10}O_2$, $C_6H_{14}S_2$, $C_8H_{10}N_2O$, $C_6H_{11}ClO_2$, $C_5H_{11}Br$, $C_{11}H_{18}$, $C_8H_{14}N_2$, $C_9H_{10}S$, $C_8H_6O_3$, $C_7H_6N_2S$, $C_6H_{14}O_4$, $C_6H_{14}O_2S$, $C_6H_6N_4O$, $C_6H_2F_4$, C_3F_6, $C_2H_2Cl_3F$
151[2]	(see m/z 137) $C_7H_5NO_3$
152	(see m/z 138) C_8H_5ClO, $C_6H_{10}Cl_2$, CCl_4
153	(see m/z 139) $C_9H_{15}NO$, C_7H_5ClNO
154	(see m/z 140; $C_{10}H_8O$ has highest occurrence of data base) C_8H_7ClO, C_2ClO, C_2ClF_5, $C_8H_{10}OS$
155	(see m/z 141) $C_8H_{13}NS$
156	(see m/z 142) $C_7H_5ClO_2$, C_6H_5Br, $C_6H_4O_5$
157	(see m/z 143) C_5H_4BrN
158	(see m/z 144) CF_6S
159	(see m/z 145) $C_6H_9NS_2$, $C_5H_6ClN_3O$
160	(see m/z 146) $C_7H_{20}Si_2$, C_6H_9Br, $C_5H_{16}Si_3$
161	(see m/z 147) $C_6H_5Cl_2N$
162	(see m/z 148) $C_{10}H_7Cl$, $C_8H_6N_2S$, $C_6H_{11}Br$, C_4F_6, $C_6H_4Cl_2O$, $CHBrCl_2$
163	(see m/z 149) $C_7H_9N_5$, C_3H_2BrNS, CCl_3NO_2
164	(see m/z 150) C_9H_8OS, $C_8H_8N_2O_2$, $C_6H_5ClN_2$, $C_7H_{16}O_4$, $C_6H_4N_4O_2$, C_5H_9BrO, $C_5H_8O_2S_2$, C_2Cl_4, $CBrClF_2$
165	(see m/z 137, 151) $C_6H_7N_5O$
166	(see m/z 138, 152) $C_{13}H_{10}$, $C_8H_6O_4$, $C_8H_6O_2S$, $C_8H_6S_2$, $C_6H_6N_4O_2$, $C_6H_6N_4S$, $C_3H_6N_2O_6$, C_3ClF_5, C_3F_6O
167	(see m/z 139, 153) $C_7H_{13}N_5$, $C_7H_5NO_4$, $C_7H_5NS_2$
168	(see m/z 140, 154) $C_{13}H_{12}$, $C_9H_{16}N_2O$, $C_8H_8O_4$, $C_8H_8O_2S$, $C_8H_8S_2$, $C_6H_4N_2O_4$, C_6HF_5, C_3H_5I, $C_2HCl_3F_2$, Cl_4Si
169	(see m/z 141, 155) C_8H_8ClNO, $C_7H_7NO_2S$
170	(see m/z 142, 156) $C_9H_{16}NO_2$, $C_8H_{10}S_2$, $C_3H_6S_4$, $C_2Cl_2F_4$, C_2F_6S
171	(see m/z 143, 157) $C_7H_9NO_2S$, $C_6H_9N_3O_3$, $C_5H_2ClN_3S$
172	(see m/z 144, 158) $C_{12}H_9F$, $C_8H_6Cl_2$, $C_8H_9ClO_2$, $C_7H_8O_3S$, $C_6H_8N_2O_2S$, C_6H_5BrO, $C_6H_4O_6$, CH_2Br_2
	(see m/z 145, 159) C_6H_4ClNOS, $C_5H_8ClN_5$
173	(see m/z 146, 160) $C_{11}H_{10}S$, $C_{10}H_6O_3$, $C_{10}H_6OS$, $C_9H_6N_2O_2$, C_6H_4BrF,
174	C_5F_6
175	(see m/z 147, 161) $C_8H_5N_3O_2$, $C_5H_9N_3S_2$, $C_7H_{10}ClNO_2$

1. Compositions are listed by m/z value, ranked in decreasing order of Occurrence probability for compounds in the *Registry of Mass Spectral Data* (Stenhagen *et al.* 1974). Only the more probable combinations of the elements H, C, N, O, F, Si, P, S, Cl, Br and I are included. Note that these are odd-electron ion compositions; many common even-electron fragment ions have compositions differing by ± 1 hydrogen atom, and can therefore be found ±1 mass unit from those listed. The above table can also be used to suggest possible elemental compositions of fragment ions
2. For masses above 150 the only compositions included are those for which a corresponding composition differing by a CH_2 less unit.

Chapter 5

Units and Measurements

5.1 Fundamental Physical Constants

Table 5.1. Physical Constants

Symbol	Name	Value	Units
amu	Atomic Mass Unit	$1.6605655 \times 10^{-24}$	g
N_o	Avogadro's Number	6.022045×10^{23}	units/mole
K	Boltzman's Constant	1.380663×10^{-16}	erg/°K
e	Electron Charge	$1.6021892 \times 10^{-19}$	coulomb
m_e	Electron Rest Mass	9.109534×10^{-28}	g
		5.485803×10^{-4}	amu
eV	Electron Volt	1.60×10^{-19}	joule
F	Faraday's Constant	9.648456×10^{4}	coulombs/equiv
		2.8925342×10	cal/volt
R	Gas Constant	8.2056×10^{-2}	1atm/°K-mole
		8.3144	joules/°K-mole
		8.3144×10^{7}	erg/°K-mole
		1.9872	cal/°K-mole
m_n	Neutron Rest Mass	$1.6749543 \times 10^{-24}$	g
		1.0086650	amu
h	Planck's Constant	6.626176×10^{-27}	erg/sec
m_p	Proton Rest Mass	$1.6726485 \times 10^{-24}$	g
		1.0072674	amu
R*	Rydberg Constant	1.0973718×10^{5}	cm
c	Speed of Light (in vacuum)	2.9979246×10^{10}	cm/sec
atm	Standard Pressure	101.3	kPa
		760	mmHg

5.2 Units

5.2.1 Base SI Units

Table 5.2. Base SI Units

Symbol	Physical Quantity	Name of Base Unit
m	Length	Meter
kg	Mass	Kilogram
s	Time	Second
A	Electric Current	Ampere
K	Thermodynamic Temperature	Kelvin
mol	Amount of Substance	Mole
cd	Luminous Intensity	Candela

5.2.2 Derived SI Units

Table 5.3. Common Derived SI Units

Symbol	Physical Quantity	Name of Unit	Definition of Unit
Å	length	Angstrom	10^{-10}m
μ	length	Micron	10^{-6}m
dyn	force	Dyne	10^{-5}N
bar	pressure	Bar	10^{-5}N · m^{-2}
erg	energy	Erg	10^{-7}J

Table 5.4. Derived SI Units with Special Names

Symbol	Physical Quantity	Name of Unit	Definition of Unit
Hz	frequency	Hertz	1/s
J	energy	Joule	N · m
N	force	Newton	kg · m/s^2
W	power	Watt	J/s
Pa	pressure	Pascal.	N/m^2
C	electric charge	Coulomb	A s
V	difference	Volt	W/A
Ohm	electrical resistance	Ohm	V/A

5.2.3 Non SI Units

Table 5.5. Non SI Units

Symbol	Physical Quantity	Name of Unit	Definition of Unit
in	length	inch	2.54 · 10^{-2} m
lb	mass	pound	0.45359237 kg
kgf	force	kilogram-force	9.80665 N
atm	pressure	atmosphere	101.325 N · m^{-2}
torr	pressure	torr	(101.325/760)N · m^{-2}
BTU	energy	British Thermal Unit	1055.056 J
kW	energy	kilowatt-hour	3.6 x 106 J
cal_{th}	energy	thermochemical calorie	4.184 J

Table 5.5. (Continued)

eV	energy	electron Volt	$1.60219 \cdot 10^{-19}$ J
amu	mass	atomic mass unit	$1.6605655 \cdot 10^{-27}$ kg
D	electric dipole moment	Debye	$3.3356 \cdot 10^{-30}$ A · m · s
F	charge per molecule	Faraday	$9.648456 \cdot 10^{4}$ C mol^{-1}

5.3 Prefixes

5.3.1 SI Prefixes

Table 5.6. SI Prefixes

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

5.3.2 Greek Prefixes

Table 5.7. Greek Prefixes

Value	Prefix
1	mono
2	di
3	tri
4	tetra
5	penta
6	hexa
7	hepta
8	octa
9	ennea
10	deca

5.4 Conversion Factors

5.4.1 Linear Conversion

1 inch = 2.5400 centimeters
1 foot = 0.3048 meter
1 yard = 0.9144 meter
1 mile = 1.6093 kilometers

1 centimeter = 0.3937 inch
1 meter = 3.281 feet
1 meter = 1.0936 yards
1 kilometer = 0.62137 miles

5.4.2 Area Conversion

1 sq. inch = 6.4516 sq. centimeters
1 sq. foot = 0.0929 sq. meter
1 sq. yard = 0.8361 sq. meter
1 sq. mile = 2.59 sq kilometers

1 sq. centimeter = 0.155 sq. inch
1 sq. meter = 10.764 sq. feet
1 sq. meter = 1.196 sq. yards
1 sq. kilometers = 0.3861 sq. mile

5.4.3 Cubic Conversion

1 cu. inch = 16.3872 cu. centimeters
1 cu. foot = 28.3 17 cu. centimeters
1 cu. yard = 0.7645 cu. meter

1 cu. centimeter = 0.0610 cu. inch
1 cu. decimeter = 0.0353 cu. foot
1 cu. meter = 1.3079 cu. yards

5.4.4 Capacity Conversion

1 fluid ounce = 29.5730 milliliters
1 liquid pint = 0.4732 liter
1 liquid quart = 0.9463 liter
1 gallon = 3.7853 liters
1 dry quart = 1.1012 liters

1 milliliter = 0.0338 fluid ounce
1 liter = 2.1134 fluid pints
1 liter = 1.0567 liquid quarts
1 liter = 0.2642 gallon
1 liter = 0.908 1 dry quart

5.4.5 Weight Conversion

1 ounce = 28.350 grams
1 pound = 0.4536 kilograms

1 gram = 0.0353 ounce
1 kilogram = 2.2046 pounds

5.4.6 Temperature Conversion

Temperature given in	To Convert to °C	To Convert to K	To Convert to °F
°C	°C	°C + 273.15	1.8 °C + 32
K	K - 273.15	K	1.8K - 459.4
°F	0.556 °F - 17.8	0.556 °F + 255.3	°F

Chapter 6

Mathematical Concepts

6.1 Algebraic Formulas

6.1.1 Laws of Exponents

$x^m \cdot x^n = x^{m+n}$ $\qquad$ $x^m \div x^n = x^{m-n}$

$(x^m)^n = x^{m \cdot n}$ $\qquad$ $(x \cdot y)^m = x^m \cdot y^m$

$(x/y)^m = x^m/y^m$ $\qquad$ $x^0 = 1$

$x^{1/n} = \sqrt[n]{x}$ $\qquad$ $x^{-m} = 1/x^m$

6.1.2 Laws of Logarithms

$\log (A \cdot B) = \log A + \log B$ $\qquad$ $\log \frac{A}{B} = \log A - \log B$

$\log A^b = b \log A$ $\qquad$ $\log \sqrt[b]{A} = \frac{\log A}{b} = \frac{1}{b} \log A$

6.1.3 Quadratic Equation

$ax^2 + bx + c = 0$ (Where $a \neq 0$ and a, b, and c are real numbers)

If the roots of $ax^2 + bx + c = 0$ are represented by r_1 and r_2, then:

1. $r_1 = \dfrac{-b + \sqrt{b^2 - 4ac}}{2a}$ and $r_2 = \dfrac{-b - \sqrt{b^2 - 4ac}}{2a}$

2. $r_1 + r_2 = -b/a$
3. $r_1 r_2 = c/a$
4. $x^2 - (r_1 + r_2)x + r_1 r_2 = 0$

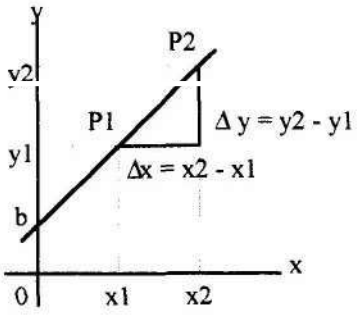
Using the discriminant to determine the nature of the roots of $ax^2 + bx + c = 0$:

5. If $b^2 - 4ac$ is zero or positive, the roots are real.
6. If $b^2 - 4ac$ is negative, the roots are imaginary.
7. If $b^2 - 4ac$ is zero, the roots are equal.
8. If $b^2 - 4ac$ is not zero, the roots are unequal.
9. If $b^2 - 4ac$ is a perfect square, the roots are rational numbers.
10. If $b^2 - 4ac$ is positive and not a perfect square, the roots are irrational numbers.

6.1.4 Graphs (a, b, c, m, and r are real numbers)

1. The slope of a line that passes through two points $P_1(x_1,y_1)$ and $P_2(x_2,y_2)$, $x1 \neq x2$:

$$m = \text{slope of } P_1P_2 = \frac{y_2 - y_1}{x_2 - x_1} = \frac{\Delta y}{\Delta x}$$



2. Equation of a straight line: $y = mx + b$ where m = slope of the line and b = y intercept.

3. Equation of a parabola: $y = ax^2 + bx + c$ or $x = ay^2 + by = c$, $a \neq 0$.

4. Equation of a circle: $(x-h)^2 + (y-k)^2 = r^2$ where the center is (h,k) and the radius is r, $r > 0$.

5. Equation of a circle: $x^2 + y^2 = r^2$ where the center is at the origin and the radius is r, $r > 0$.

6. Equation of an ellipse: $ax^2 + by^2 = c$ where the center is at the origin; a, b, and c are positive; $c \neq 0$.

7. Equation of a hyperbola: $ax^2 - by^2 = c$, $ay^2 - bx^2 = c$ where the center is at the origin; a and b are positive. Also xy = k, k is a constant.

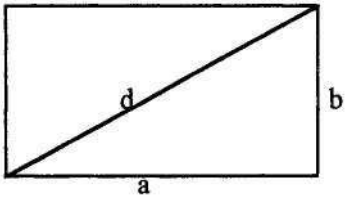
8. At the turning point of the parabola $y = ax^2 + bx + c$, $x = -b/2a$

9. The graph of the parabola $y = ax^2 + bx + c$ opens upward and has a minimum turning point when a is positive, $a > 0$.

10. The graph of the parabola $y = ax^2 + bx + c$ opens downward and has a maximum turning point when a is negative, $a < 0$.

6.2 Plane Figure Formulas

6.2.1 Rectangle



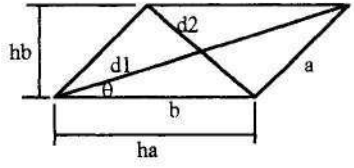
Area A = ab

Perimeter P = 2 (a + b)

Diagonal $d = \sqrt{a^2 + b^2}$

If a = b then it is a square

6.2.2 Parallelogram



Area $A = ah_a = bh_b = ab \sin \theta$

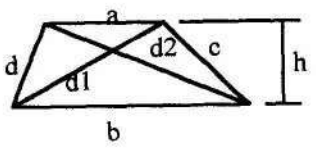
Perimeter P = 2 (a + b)

Diagonal:

$d1 = \sqrt{a^2 + b^2 - 2ab \cos \theta}$

$d2 = \sqrt{a^2 + b^2 + 2ab \cos\theta}$

6.2.3 Trapezoid



Area $A = \frac{(a+b)\,h}{2}$

Perimeter $P = a + b + c + d$

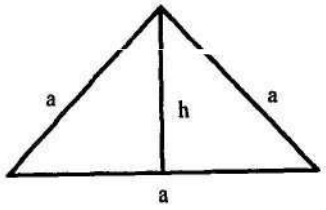
Diagonal $= d_1 = \sqrt{ab + \frac{ac^2 - bd^2}{a-b}}$

$$d_2 = \sqrt{ab + \frac{ad^2 - bc^2}{a-b}}$$

Height $= h = \frac{2}{a-b} \cdot \sqrt{s(s-a+b)(s-c)(s-d)}$

where $s = \frac{1}{2}(a - b + c + d)$

6.2.4 Equilateral Triangle



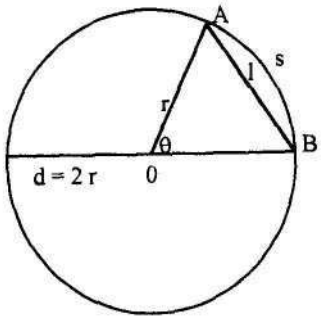
a = all sides equal

Area $A = a^2 \frac{\sqrt{3}}{4} = 0.433\ a^2$

Perimeter $P = 3\ a$

$h = \frac{\sqrt{3}}{2}\ a = 0.866\ a$

6.2.5 Circle



Area of circle $A = \pi r^2 = 3.14159\ r^2$

$= \pi \frac{d^2}{4} = 0.78539\ d$

Area of sector $AsB0A = \frac{\pi \theta r^2}{360}$

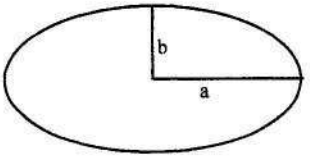
Area of segment $AsBlA = \frac{\pi r^2 \theta}{360} - \frac{r^2 \sin \theta}{2}$

Circumference $= 2\ \pi\ r = 6.28318\ r$

$= \pi\ d = 3.14159\ d$

Length of chord $AlB = 2\ r \sin \frac{\theta}{2}$ Length of arc $AsB = \frac{\pi r \theta}{180}$

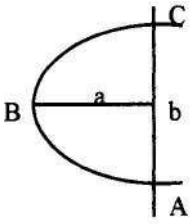
6.2.6 Ellipse



Area $A = \pi ab = 3.14159\ a\ b$

Circumference $\approx 2\pi\sqrt{\frac{a^2+b^2}{2}}$

6.2.7 Parabola

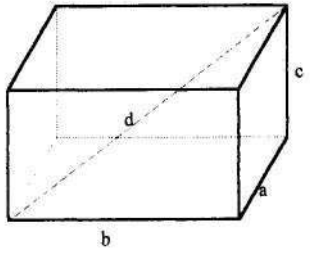


Area ABCA =2/3 a b

Length of arc ABC $= b\ \{½\ (1 + 16\ (a/b)^2)^{½} + \frac{1}{8\ (\frac{a}{b})}\ \ln\ [4\ n + (1 + 16\ (a/b)^2)^{½}]\}$

6.3 Solid Figure Formulas

6.3.1 Parallelpiped



Surface area $A = 2\ (ab + bc + ca)$

Volume $V = abc$

Diagonal $d = \sqrt{a^2 + b^2 + c^2}$

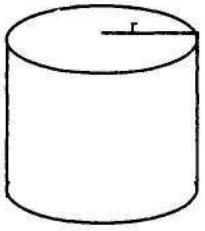
In the case of a cube, $a = b = c$ then;

Surface $= 6\ a^2$

Volume $V = a^3$

Diagonal $d = a\sqrt{3}$

6.3.2 Right Cylinder



Surface area of convex surface $A_c = 2 \pi r h$

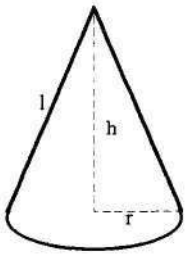
$= 6.283 r h$

Total surface area $A = 2 \pi r (r + h)$

Volume $V = \pi r^2 h$

6.3.3 Right Cone

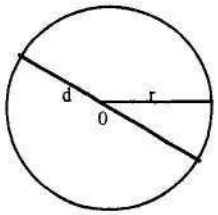
Surface area of convex surface $A_c = \pi r l$



(l = slant height = $\sqrt{r^2 - h^2}$)

Total surface area $A = \pi r (r + l)$

Volume $V = 1/3 \pi r^2 h$



6.3.4 Sphere

Surface area $A = 4 \pi r^2 = \pi d^2$

Volume $V = 4/3 \pi r^3 = 1/6 \pi d^3$

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