2 Summary Tables

2.1
General Tables

2.1.1
Calculation of the Number of Double Bond Equivalents from the Molecular Formula

General Equation:

$$\text{double bond equivalents} = \frac{2 + \sum_i n_i (v_i - 2)}{2}$$

n_i: number of atoms of element i in molecular formula
v_i: formal valence of element i

Short Cut:

For compounds containing only C, H, O, N, S, and halogens, the following steps permit a quick and simple calculation of the number of double bond equivalents:

1. O and divalent S are deleted from the molecular formula
2. Halogens are replaced by hydrogen
3. Trivalent N is replaced by CH
4. The resulting hydrocarbon, C_nH_x, is compared with the saturated hydrocarbon, C_nH_{2n+2}. Each double bond equivalent reduces the number of hydrogen atoms by 2:

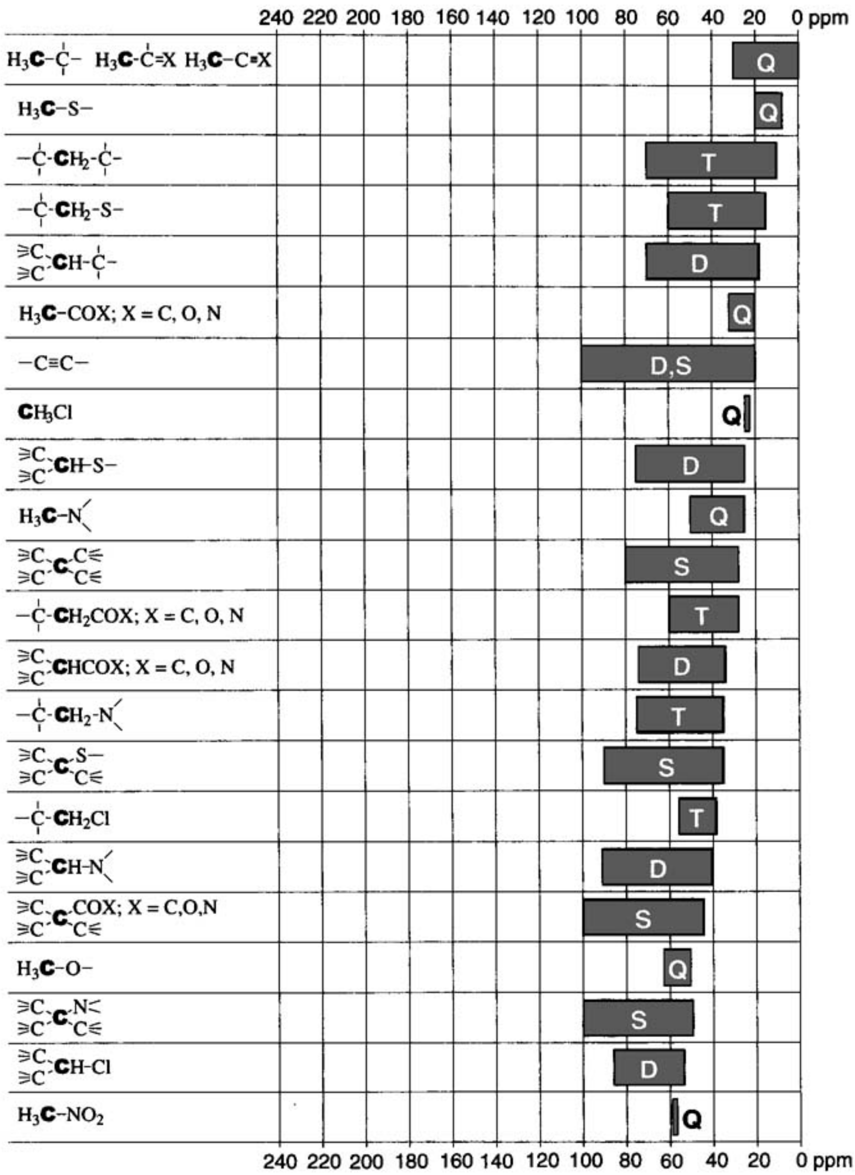
$$\text{double bond equivalents} = \frac{2n + 2 - x}{2}$$

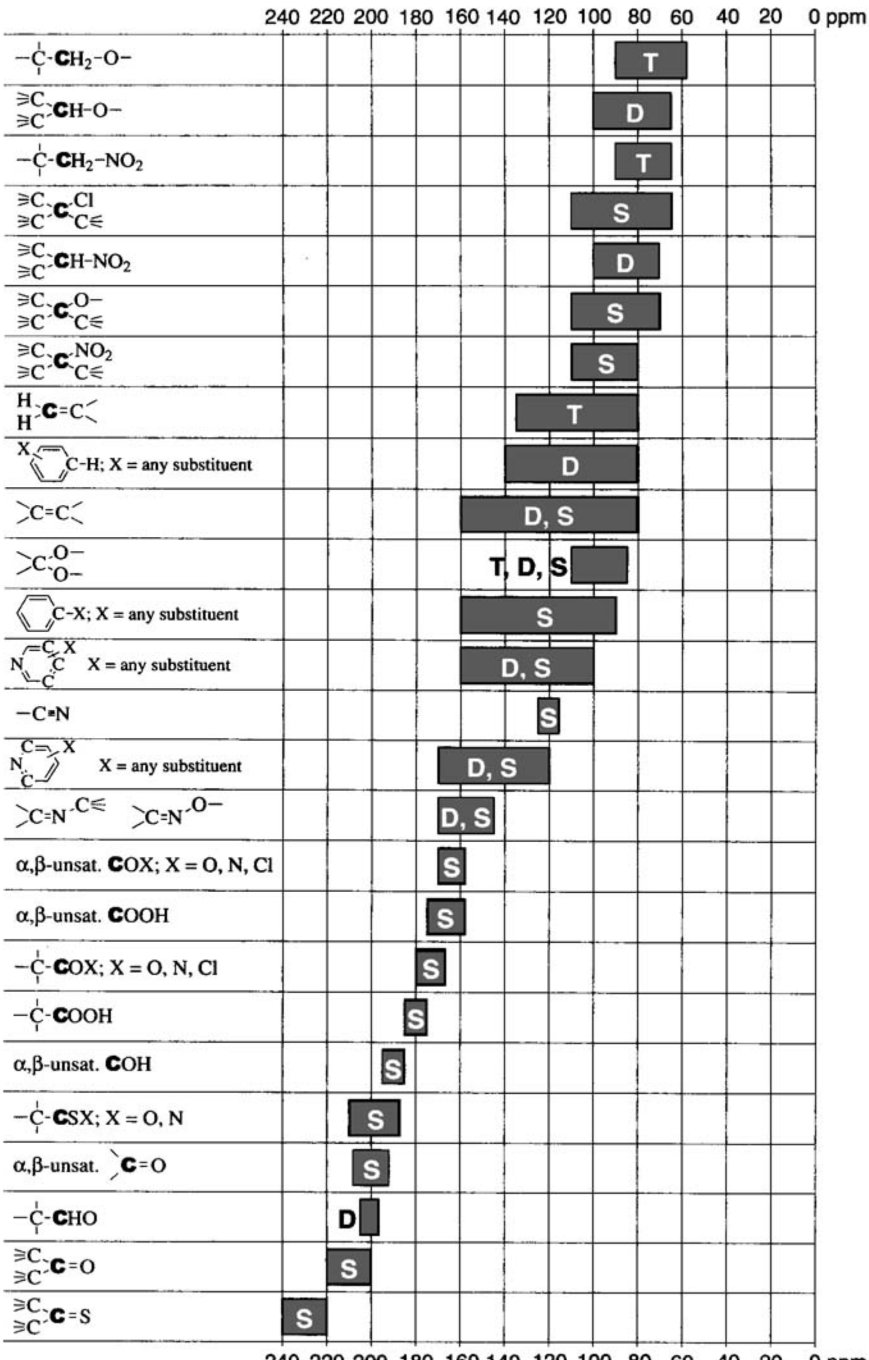
2.1.2
Properties of Selected Nuclei

Isotope	Natural abundance [%]	Spin quantum number, I	Frequency [MHz] at 2.35 Tesla	Relative sensitivity of nucleus	Relative sensitivity at natural abundance	Electric quadrupole moment [e × 10^{-24} cm^2]
^{1}H	99.985	1/2	100.0	1	1	
^{2}H	0.015	1	15.4	9.6×10^{-3}	1.5×10^{-6}	2.8×10^{-3}
^{3}H	0.000	1/2	106.7	1.2	0	
^{10}B	19.58	3	10.7	2.0×10^{-2}	3.9×10^{-3}	7.4×10^{-2}
^{11}B	80.42	3/2	32.1	1.6×10^{-1}	1.3×10^{-1}	3.6×10^{-2}
^{13}C	1.108	1/2	25.1	1.6×10^{-2}	1.8×10^{-4}	
^{14}N	99.635	1	7.3	1.0×10^{-3}	1.0×10^{-3}	1.9×10^{-2}
^{15}N	0.365	1/2	10.1	1.0×10^{-3}	3.8×10^{-6}	
^{17}O	0.037	5/2	13.6	2.9×10^{-2}	1.1×10^{-5}	-2.6×10^{-2}
^{19}F	100.000	1/2	94.1	8.3×10^{-1}	8.3×10^{-1}	
^{31}P	100.000	1/2	40.5	6.6×10^{-2}	6.6×10^{-2}	
^{33}S	0.76	3/2	7.6	2.3×10^{-3}	1.7×10^{-5}	-6.4×10^{-2}
^{117}Sn	7.61	1/2	35.6	4.5×10^{-2}	3.4×10^{-3}	
^{119}Sn	8.58	1/2	37.3	5.2×10^{-2}	4.4×10^{-3}	
^{195}Pt	33.8	1/2	21.5	9.9×10^{-3}	3.4×10^{-3}	
^{199}Hg	16.84	1/2	17.8	5.7×10^{-3}	9.5×10^{-4}	
^{207}Pb	22.6	1/2	20.9	9.2×10^{-3}	2.1×10^{-4}	

2.2
^{13}C NMR Spectroscopy

Summary of the Regions of Chemical Shifts, δ, for Carbon Atoms in Various Chemical Environments *(δ in ppm relative to TMS. Carbon atoms are specified as follows: Q for CH_3, T for CH_2, D for CH, and S for C).*




240 220 200 180 160 140 120 100 80 60 40 20 0 ppm
X = any substituent
α,β-unsat. COX; X = O, N, Cl
α,β-unsat. COOH
α,β-unsat. COH
α,β-unsat. C=O
T
D
S
D, S
T, D, S
240 220 200 180 160 140 120 100 80 60 40 20 0 ppm

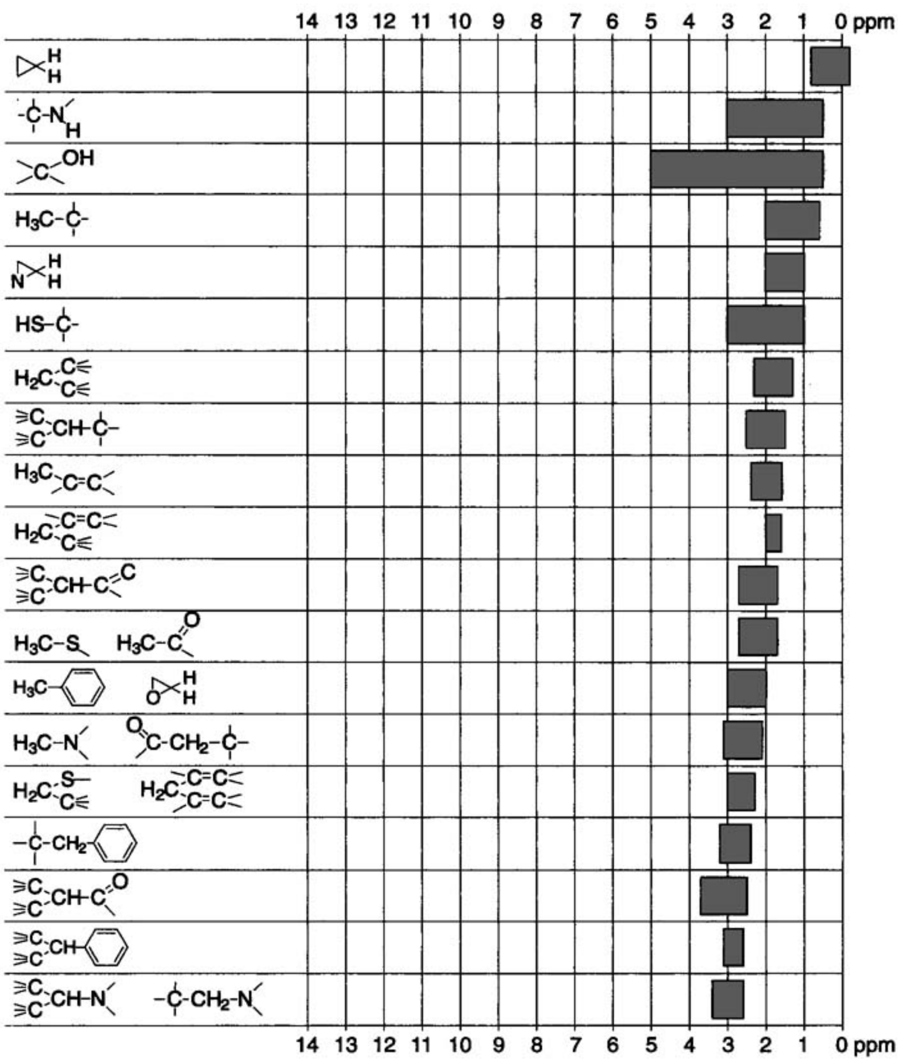
^{13}C Chemical Shifts for Carbonyl Groups (δ in ppm relative to TMS)

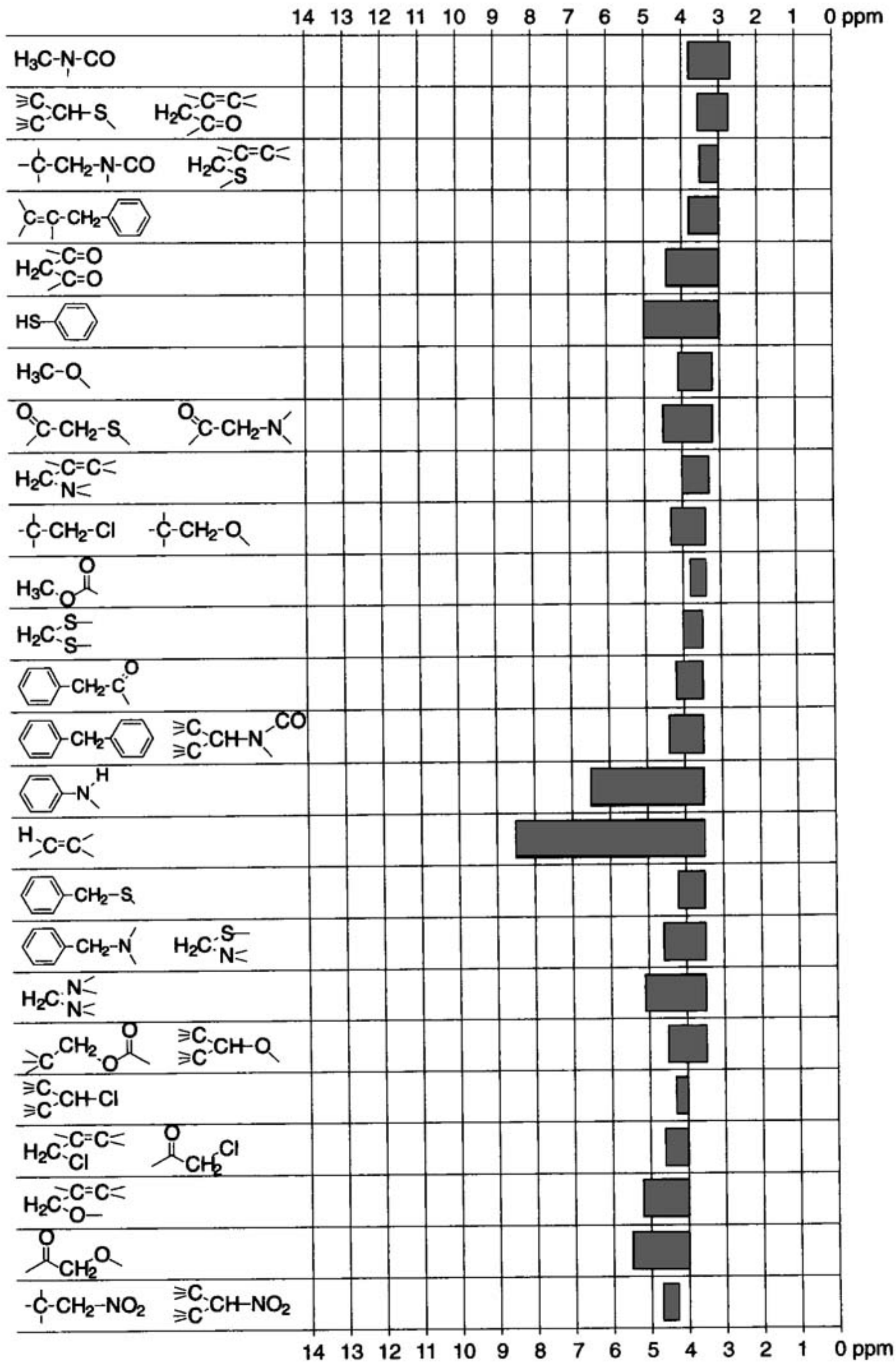
R	R–CHO	R–$COCH_3$	R–COOH	R–COO^-
–H	197.0	200.5	166.3	171.3
–CH_3	200.5	206.7	176.9	182.6
–CH_2CH_3	202.7	207.6	180.4	185.1
–$CH(CH_3)_2$	204.6	211.8	184.1	
–$C(CH_3)_3$	205.6	213.5	185.9	188.6
–*n*-C_8H_{17}	202.6	207.9	180.7	183.1
–CH_2Cl	193.3	200.1	173.7	175.9
–$CHCl_2$		193.6	170.4	171.8
–CCl_3	176.9	186.3	167.1	167.6
–cyclohexyl	204.7	209.4	182.1	185.4
–CH=CH_2	194.4	197.5	171.7	174.5
–C≡CH	176.8		156.5	
–phenyl	192.0	196.9	172.6	177.6

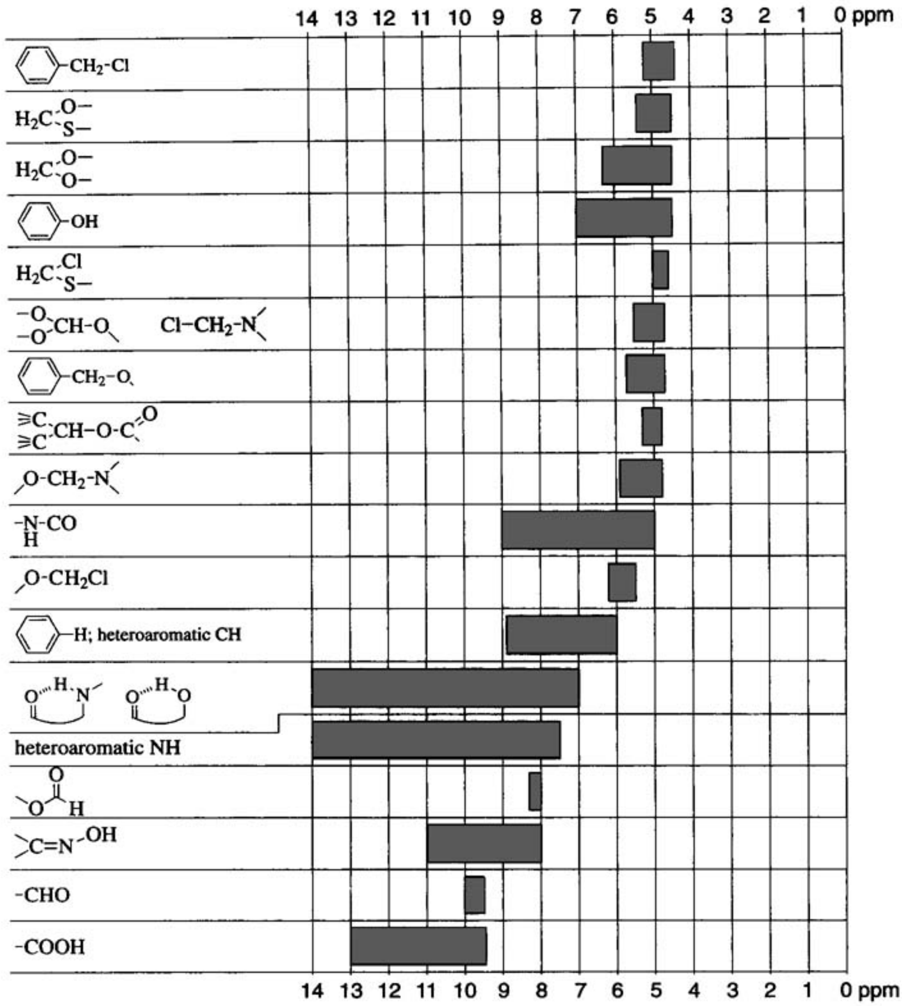
R	R–$COOCH_3$	R–$CONH_2$	R–COOCO–R	R–COCl
–H	161.6	167.6	158.5	
–CH_3	171.3	173.4	167.4	170.4
–CH_2CH_3	173.3	177.2	170.3	174.7
–$CH(CH_3)_2$	177.4		172.8	178.0
–$C(CH_3)_3$	178.8	180.9	173.9	180.3
–*n*-C_8H_{17}	174.4	176.3	169.4	173.8
–CH_2Cl	167.8	168.3	162.1	167.7
–$CHCl_2$	165.1		157.6	165.5
–CCl_3	162.5		154.1	
–cyclohexyl	175.3	177.3		176.3
–CH=CH_2	166.5	168.3		165.6
–C≡CH	153.4			
–phenyl	166.8	169.7	162.8	168.0

2.3
¹H NMR Spectroscopy

Summary of the Regions of Chemical Shifts for Hydrogen Atoms in Various Chemical Environments *(δ in ppm relative to TMS)*

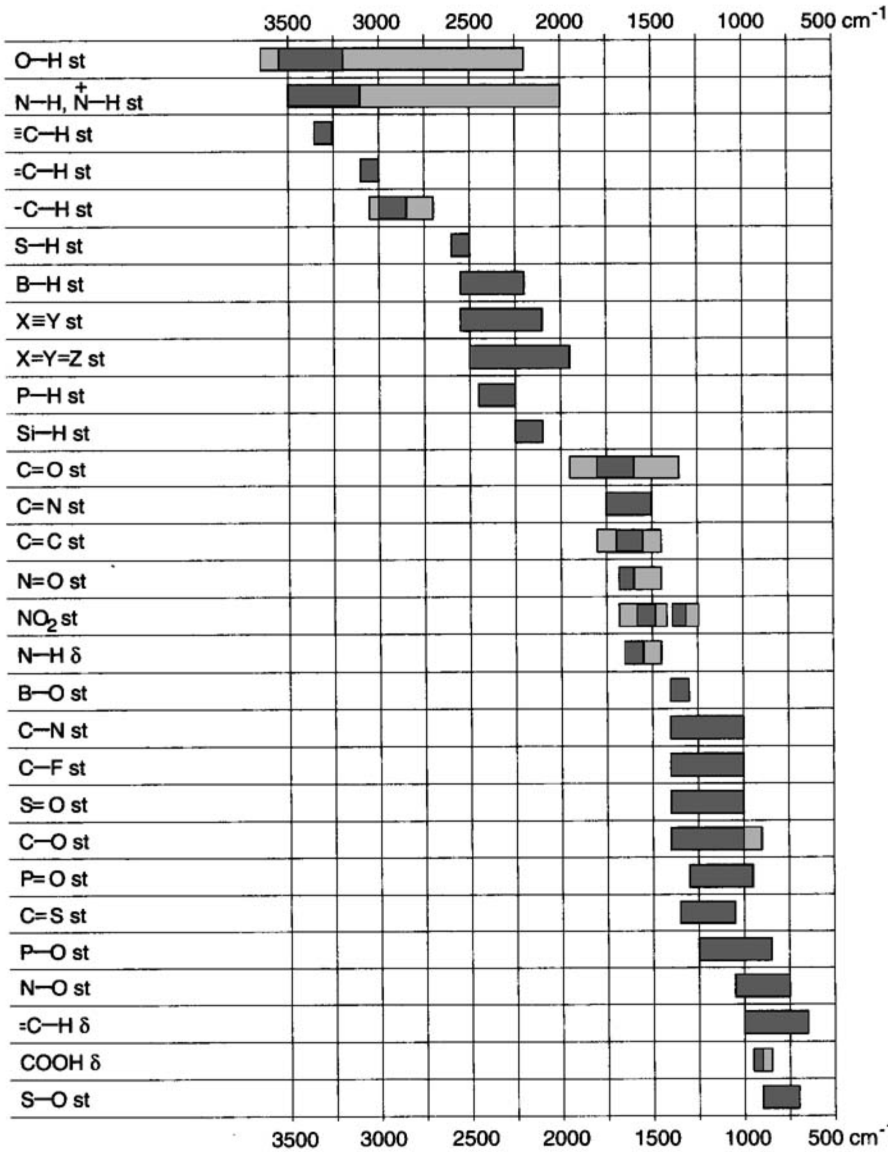



14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

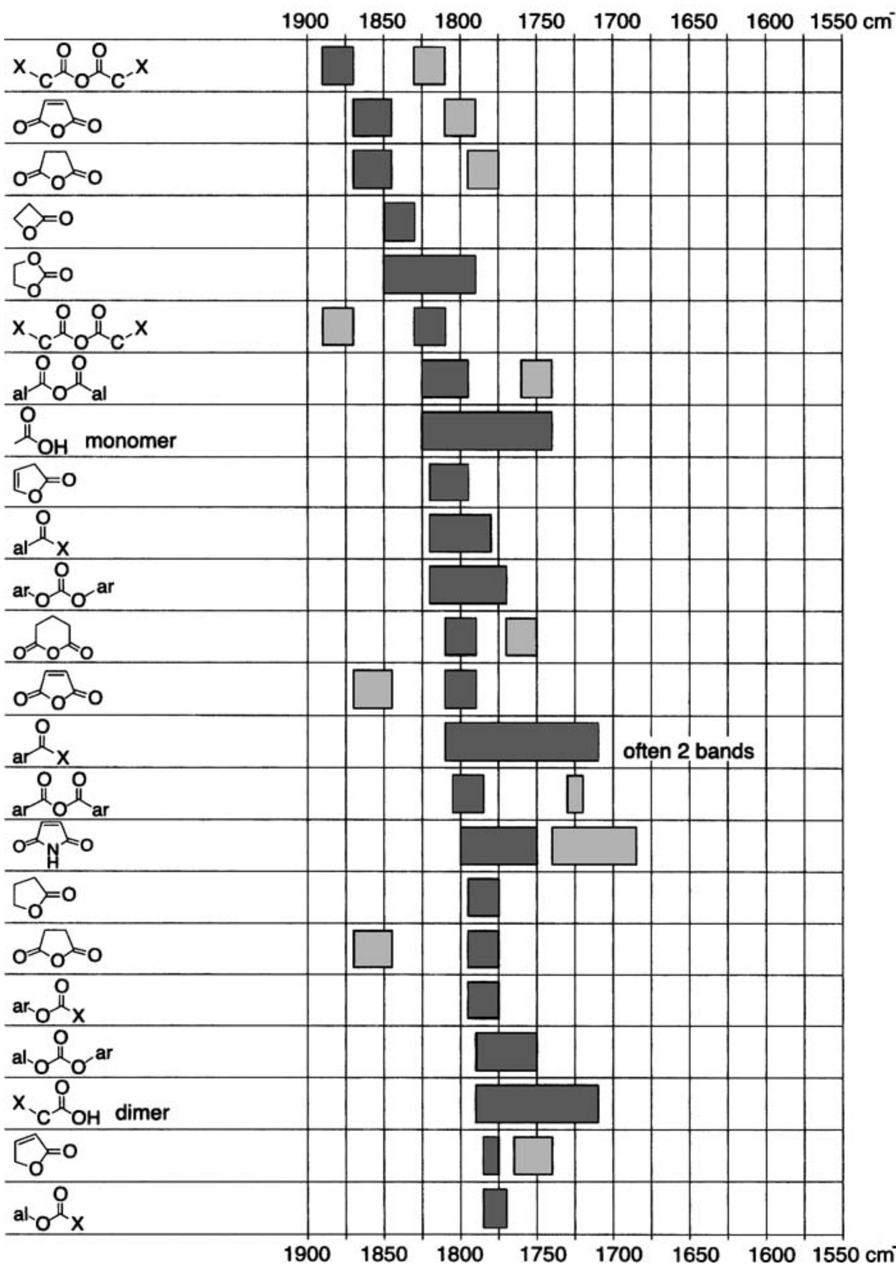

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
-CH2-Cl
-OH
Cl-CH2-N
-CH2-O
-N-CO
H
O-CH2Cl
-H; heteroaromatic CH
heteroaromatic NH
C=N-OH
-CHO
-COOH
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

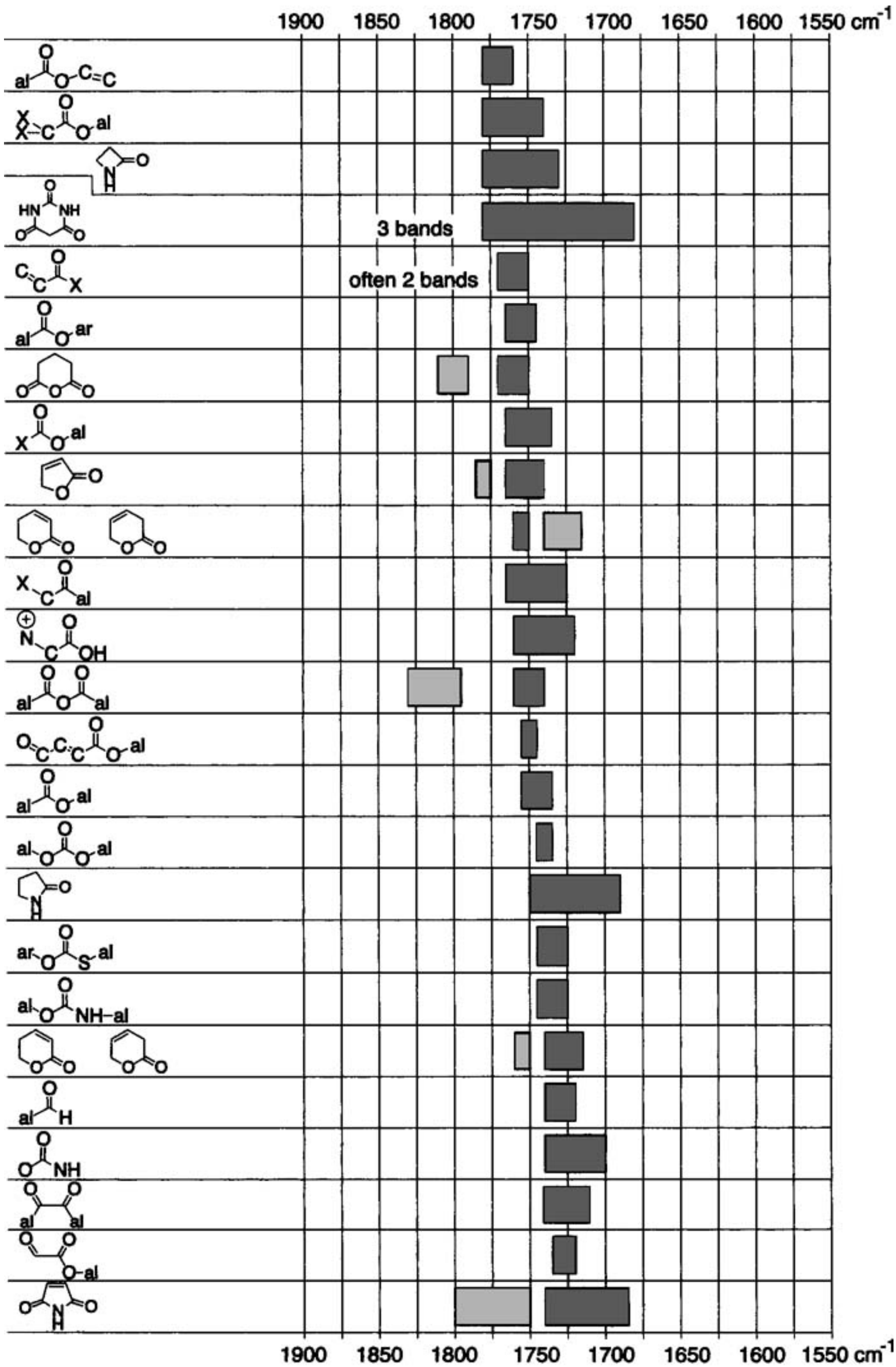
2.4
IR Spectroscopy

Summary of the Most Important IR Absorption Bands

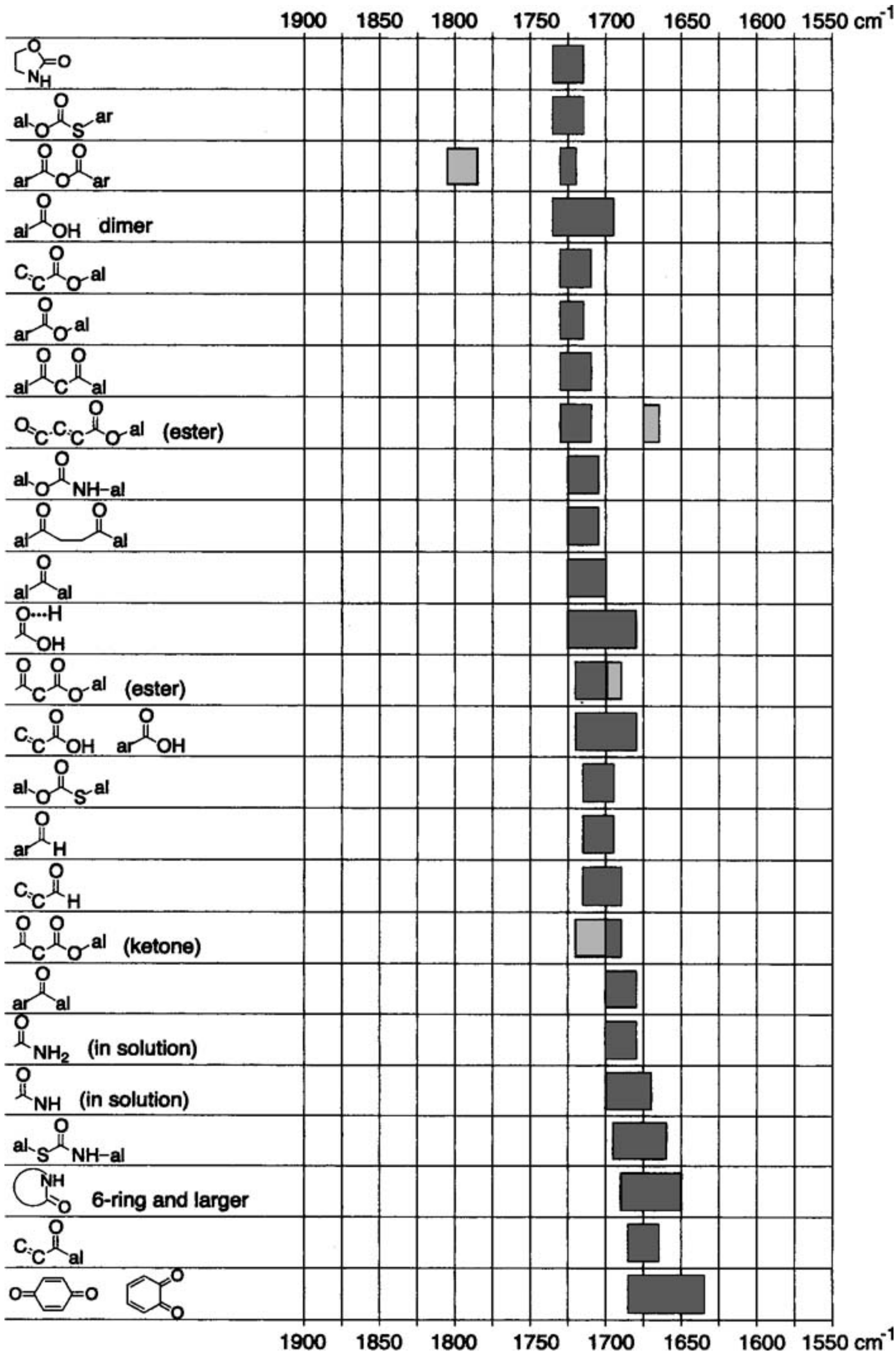


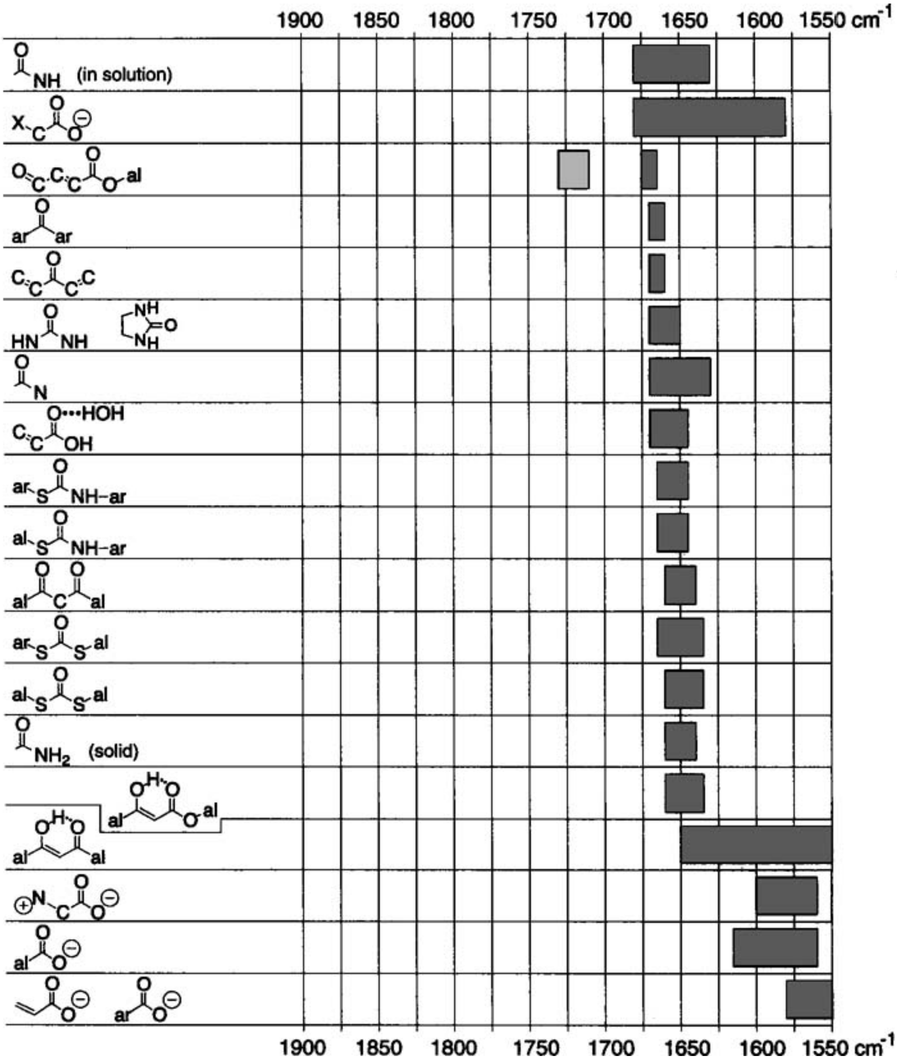
Summary of IR Absorption Bands of Carbonyl Groups (in cm^{-1})





1900 1850 1800 1750 1700 1650 1600 1550 cm⁻¹
3 bands
often 2 bands


1900 1850 1800 1750 1700 1650 1600 1550 cm⁻¹
al O S ar
ar O ar
al OH dimer
C C O al
ar O al
al C al
O C C C O al (ester)
al O NH–al
al al
al al
O···H
OH
C O al (ester)
C C OH ar OH
al O S al
ar H
C C H
C O al (ketone)
ar al
NH2 (in solution)
NH (in solution)
al S NH–al
NH
6-ring and larger
C C al
1900 1850 1800 1750 1700 1650 1600 1550 cm⁻¹


1900 1850 1800 1750 1700 1650 1600 1550 cm⁻¹
(in solution)
(solid)

2.5 Mass Spectrometry

2.5.1 Average Masses of Naturally Occurring Elements with Exact Masses and Representative Relative Abundances of Isotopes [1–3]

Element Isotope	Mass	Abundance
H	1.00795[a]	
^{1}H	1.007825	100[b]
^{2}H	2.014101	0.0115 (in water)
He	4.002602[a]	
^{3}He	3.016029	0.000137
^{4}He	4.002603	100 (in air)
Li	6.941[a]	
^{6}Li	6.015122	8.21[c]
^{7}Li	7.016004	100
Be	9.012182	
^{9}Be	9.012182	100
B	10.812[a]	
^{10}B	10.012937	24.8[b]
^{11}B	11.009306	100
C	12.0108[a]	
^{12}C	12.000000	100
^{13}C	13.003355	1.08
N	14.00675[a]	
^{14}N	14.003070	100
^{15}N	15.000109	0.369
O	15.9994[a]	
^{16}O	15.994915	100
^{17}O	16.999132	0.038
^{18}O	17.999116	0.205
F	18.998403	
^{19}F	18.998403	100

Element Isotope	Mass	Abundance
Ne	20.1798[a]	
^{20}Ne	19.992402	100[b]
^{21}Ne	20.993847	0.30
^{22}Ne	21.991386	10.22 (in air)
Na	22.989769	
^{23}Na	22.989769	100
Mg	24.3051	
^{24}Mg	23.985042	100
^{25}Mg	24.985837	12.66
^{26}Mg	25.982593	13.94
Al	26.981538	
^{27}Al	26.981538	100
Si	28.0855[a]	
^{28}Si	27.976927	100
^{29}Si	28.976495	5.0778
^{30}Si	29.973770	3.3473
P	30.973762	
^{31}P	30.973762	100
S	32.067[a]	
^{32}S	31.972071	100
^{33}S	32.971459	0.80
^{34}S	33.967867	4.52
^{36}S	35.967081	0.02
Cl	35.4528	
^{35}Cl	34.968853	100[b]
^{37}Cl	36.965903	31.96

Element Isotope	Mass	Abundance
Ar	39.948[a]	
^{36}Ar	35.967546	0.3379
^{38}Ar	37.962776	0.0635
^{40}Ar	39.962383	100 (in air)
K	39.0983	
^{39}K	38.963706	100
^{40}K	39.963999	0.0125
^{41}K	40.961826	7.2167
Ca	40.078	
^{40}Ca	39.962591	100
^{42}Ca	41.958618	0.667
^{43}Ca	42.958769	0.139
^{44}Ca	43.955481	2.152
^{46}Ca	45.953693	0.004
^{48}Ca	47.952534	0.193
Sc	44.955910	
^{45}Sc	44.955910	100
Ti	47.867	
^{46}Ti	45.952629	11.19
^{47}Ti	46.951764	10.09
^{48}Ti	47.947947	100
^{49}Ti	48.947871	7.34
^{50}Ti	49.944792	7.03
V	50.9415	
^{50}V	49.947163	0.250
^{51}V	50.943964	100
Cr	51.9962	
^{50}Cr	49.946050	5.187
^{52}Cr	51.940512	100
^{53}Cr	52.940654	11.339
^{54}Cr	53.938885	2.823
Mn	54.938050	
^{55}Mn	54.938050	100
Fe	55.845	
^{54}Fe	53.939615	6.370
^{56}Fe	55.934942	100

Element Isotope	Mass	Abundance
^{57}Fe	56.935399	2.309
^{58}Fe	57.933280	0.307
Co	58.933200[a]	
^{59}Co	58.933200	100
Ni	58.6934	
^{58}Ni	57.935348	100
^{60}Ni	59.930791	38.5198
^{61}Ni	60.931060	1.6744
^{62}Ni	61.928349	5.3388
^{64}Ni	63.927970	1.3596
Cu	63.546	
^{63}Cu	62.929601	100
^{65}Cu	64.927794	44.57
Zn	65.39	
^{64}Zn	63.929147	100
^{66}Zn	65.926037	57.37
^{67}Zn	66.927131	8.43
^{68}Zn	67.924848	38.56
^{70}Zn	69.925325	1.27
Ga	69.723	
^{69}Ga	68.925581	100[b]
^{71}Ga	70.924705	66.367
Ge	72.61	
^{70}Ge	69.924250	56.44
^{72}Ge	71.922076	75.91
^{73}Ge	72.923459	21.31
^{74}Ge	73.921178	100
^{76}Ge	75.921403	20.98
As	74.921596	
^{75}As	74.921596	100
Se	78.96	
^{74}Se	73.922477	1.79
^{76}Se	75.919214	18.89
^{77}Se	76.919915	15.38
^{78}Se	77.917310	47.91
^{80}Se	79.916522	100
^{82}Se	81.916700	17.60

Element Isotope	Mass	Abundance
Br	79.904	
^{79}Br	78.918338	100
^{81}Br	80.916291	97.28
Kr	83.80	
^{78}Kr	77.920387	0.61[b]
^{80}Kr	79.916378	4.00
^{82}Kr	81.913485	20.32
^{83}Kr	82.914136	20.16
^{84}Kr	83.911507	100
^{86}Kr	85.910610	30.35
		(in air)
Rb	85.4678	
^{85}Rb	84.911789	100
^{87}Rb	86.909183	38.56
Sr	87.62[a]	
^{84}Sr	83.913425	0.68
^{86}Sr	85.909262	11.94
^{87}Sr	86.908879	8.48
^{88}Sr	87.905614	100
Y	88.905848	
^{89}Y	88.905848	100
Zr	91.224	
^{90}Zr	89.904704	100
^{91}Zr	90.905645	21.81
^{92}Zr	91.905040	33.33
^{94}Zr	93.906316	33.78
^{96}Zr	95.908276	5.44
Nb	92.906378	
^{93}Nb	92.906378	100
Mo	95.94	
^{92}Mo	91.906810	61.50
^{94}Mo	93.905088	38.33
^{95}Mo	94.905841	65.98
^{96}Mo	95.904679	69.13
^{97}Mo	96.906021	39.58
^{98}Mo	97.905408	100
^{100}Mo	99.907478	39.91

Element Isotope	Mass	Abundance
Ru	101.07	
^{96}Ru	95.907599	17.56
^{98}Ru	97.905288	5.93
^{99}Ru	98.905939	40.44
^{100}Ru	99.904229	39.94
^{101}Ru	100.905582	54.07
^{102}Ru	101.904350	100
^{104}Ru	103.905430	59.02
Rh	102.905504	
^{103}Rh	102.905504	100
Pd	106.42	
^{102}Pd	101.905608	3.73
^{104}Pd	103.904036	40.76
^{105}Pd	104.905084	81.71
^{106}Pd	105.903484	100
^{108}Pd	107.903894	96.82
^{110}Pd	109.905151	42.88
Ag	107.8682	
^{107}Ag	106.905094	100
^{109}Ag	108.904756	92.90
Cd	112.412	
^{106}Cd	105.906459	4.35
^{108}Cd	107.904184	3.10
^{110}Cd	109.903006	43.47
^{111}Cd	110.904182	44.55
^{112}Cd	111.902757	83.99
^{113}Cd	112.904401	42.53
^{114}Cd	113.903358	100
^{116}Cd	115.904755	26.07
In	114.818	
^{113}In	112.904061	4.48
^{115}In	114.903879	100
Sn	118.711	
^{112}Sn	111.904822	2.98
^{114}Sn	113.902782	2.03
^{115}Sn	114.903346	1.04
^{116}Sn	115.901744	44.63
^{117}Sn	116.902954	23.57
^{118}Sn	117.901606	74.34

(contd.)

Element Isotope	Mass	Abundance
^{119}Sn	118.903309	26.37
^{120}Sn	119.902197	100
^{121}Sn	121.903440	14.21
^{124}Sn	123.905275	17.77
Sb	121.760	
^{121}Sb	120.903818	100
^{123}Sb	122.904216	74.79
Te	127.60	
^{120}Te	119.904021	0.26
^{122}Te	121.903047	7.48
^{123}Te	122.904273	2.61
^{124}Te	123.902819	13.91
^{125}Te	124.904425	20.75
^{126}Te	125.903306	55.28
^{128}Te	127.904461	93.13
^{130}Te	129.906223	100
I	126.904468	
^{127}I	126.904468	100
Xe	131.29	
^{124}Xe	123.905896	0.33^b
^{126}Xe	125.904270	0.33
^{128}Xe	127.903530	7.14
^{129}Xe	128.904779	98.33
^{130}Xe	129.903508	15.17
^{131}Xe	130.905082	78.77
^{132}Xe	131.904154	100
^{134}Xe	133.905395	38.82
^{136}Xe	135.907221	32.99
Cs	132.905447	
^{133}Cs	132.905447	100
Ba	137.328	
^{130}Ba	129.906311	0.148
^{132}Ba	131.905056	0.141
^{134}Ba	133.904503	3.371
^{135}Ba	134.905683	9.194
^{136}Ba	135.904570	10.954
^{137}Ba	136.905821	15.666
^{138}Ba	137.905241	100

Element Isotope	Mass	Abundance
La	138.9055	
^{138}La	137.907107	0.090
^{139}La	138.906348	100
Ce	140.116	
^{136}Ce	135.907145	0.209
^{138}Ce	137.905991	0.284
^{140}Ce	139.905434	100
^{142}Ce	141.909240	12.565
Pr	140.907648	
^{141}Pr	140.907648	100
Nd	144.24	
^{142}Nd	141.907719	100
^{143}Nd	142.909810	44.9
^{144}Nd	143.910083	87.5
^{145}Nd	144.912569	30.5
^{146}Nd	145.913112	63.2
^{148}Nd	147.916889	21.0
^{150}Nd	149.920887	20.6
Sm	150.36	
^{144}Sm	143.911995	11.48
^{147}Sm	146.914893	56.04
^{148}Sm	147.914818	42.02
^{149}Sm	148.917180	51.66
^{150}Sm	149.917271	27.59
^{152}Sm	151.919728	100
^{154}Sm	153.922205	85.05
Eu	151.964	
^{151}Eu	150.919846	91.61
^{153}Eu	152.921226	100
Gd	157.25	
^{152}Gd	151.919788	0.81
^{154}Gd	153.920862	8.78
^{155}Gd	154.922619	59.58
^{156}Gd	155.922120	82.41
^{157}Gd	156.923957	63.00
^{158}Gd	157.924101	100
^{160}Gd	159.927051	88.00
Tb	158.925343	
^{159}Tb	158.925343	100

Element Isotope	Mass	Abundance
Dy	162.50	
^{156}Dy	155.924279	0.21
^{158}Dy	157.924405	0.35
^{160}Dy	159.925194	8.30
^{161}Dy	160.926930	67.10
^{162}Dy	161.926795	90.53
^{163}Dy	162.928728	88.36
^{164}Dy	163.929171	100
Ho	164.930319	
^{165}Ho	164.930319	100
Er	167.26	
^{162}Er	161.928775	0.42
^{164}Er	163.929197	4.79
^{166}Er	165.930290	100
^{167}Er	166.932045	68.22
^{168}Er	167.932368	79.69
^{170}Er	169.935460	44.42
Tm	168.934211	
^{169}Tm	168.934211	100
Yb	173.04	
^{168}Yb	167.933894	0.41
^{170}Yb	169.934759	9.55
^{171}Yb	170.936322	44.86
^{172}Yb	171.936378	68.58
^{173}Yb	172.938207	50.68
^{174}Yb	173.938858	100
^{176}Yb	175.942568	40.09
Lu	174.967	
^{175}Lu	174.940768	100
^{176}Lu	175.942682	2.66
Hf	178.49	
^{174}Hf	173.940040	0.46
^{176}Hf	175.941402	14.99
^{177}Hf	176.943220	53.02
^{178}Hf	177.943698	77.77
^{179}Hf	178.944815	38.83
^{180}Hf	179.946549	100
Ta	180.9479	
^{180}Ta	179.947466	0.012

Element Isotope	Mass	Abundance
^{181}Ta	180.947996	100
W	183.84	
^{180}W	179.946707	0.40
^{182}W	181.948206	86.49
^{183}W	182.950224	46.70
^{184}W	183.950933	100
^{186}W	185.954362	93.79
Re	186.207	
^{185}Re	184.952956	59.74
^{187}Re	186.955751	100
Os	190.23	
^{184}Os	183.952491	0.05
^{186}Os	185.953838	3.90
^{187}Os	186.955748	4.81
^{188}Os	187.955836	32.47
^{189}Os	188.958145	39.60
^{190}Os	189.958445	64.39
^{192}Os	191.961479	100
Ir	192.217	
^{191}Ir	190.960591	59.49
^{193}Ir	192.962924	100
Pt	195.078	
^{190}Pt	189.959931	0.041
^{192}Pt	191.961035	2.311
^{194}Pt	193.962664	97.443
^{195}Pt	194.964774	100
^{196}Pt	195.964935	74.610
^{198}Pt	197.967876	21.172
Au	196.966552	
^{197}Au	196.966552	100
Hg	200.59	
^{196}Hg	195.965815	0.50
^{198}Hg	197.966752	33.39
^{199}Hg	198.968262	56.50
^{200}Hg	199.968309	77.36
^{201}Hg	200.970285	44.14
^{202}Hg	201.970626	100
^{204}Hg	203.973476	23.00

Element Isotope	Mass	Abundance
Tl	204.3833	
^{203}Tl	202.972329	41.892
^{205}Tl	204.974412	100
Pb	207.2[a]	
^{204}Pb	203.973029	2.7
^{206}Pb	205.974449	46.0
^{207}Pb	206.975881	42.2
^{208}Pb	207.976636	100
Bi	208.980383	
^{209}Bi	208.980383	100
Th	232.038050	
^{232}Th	232.038050	100
U	238.0289	
^{234}U	234.040946	0.0055[d]
^{235}U	235.043923	0.73
^{238}U	238.050783	100

[a] Natural variations in the isotopic composition of terrestrial material does not allow to give a more precise value.

[b] Commercially available materials may have substantially different isotopic compositions if they were subjected to undisclosed or inadvertent isotopic fractionation.

[c] Materials depleted in ^{6}Li are commercial sources of laboratory shelf reagents and are known to have ^{6}Li abundances in the range of 2.0007-7.672 atom percent, with natural materials at the higher end of this range. Average atomic masses vary between 6.939 and 6.996; if a more accurate value is required, it must be determined for the specific material.

[d] Materials depleted in ^{235}U are commercial sources of laboratory shelf reagents.

2.5.2 Ranges of Natural Isotope Abundances of Selected Elements [3]

Element Isotope	Range (atom %)
H	
^{1}H	99.9816–99.9975
^{2}H	0.0184–0.0025
He	
^{3}He	4.6x10^{-8}–0.0041
^{4}He	100–99.9959
Li	
^{6}Li	7.21–7.71
^{7}Li	92.79–92.29
B	
^{10}B	18.927–20.337
^{11}B	81.073– 79.663
C	
^{12}C	98.85–99.02
^{13}C	1.15–0.98
N	
^{14}N	99.890–99.652
^{15}N	0.411–0.348
O	
^{16}O	99.7384–99.7756
^{17}O	0.0399–0.0367
^{18}O	0.2217–0.1877
Ne	
^{20}Ne	90.514–88.47
^{21}Ne	1.71–0.266
^{22}Ne	9.96–9.20
Si	
^{28}Si	92.21–92.25
^{29}Si	4.69–4.67
^{30}Si	3.10–3.08
S	
^{32}S	94.537–95.261
^{33}S	0.787–0.731
^{34}S	4.655–3.993
^{36}S	0.021–0.015
Cl	
^{35}Cl	75.64–75.86
^{37}Cl	24.36–24.14
Ca	
^{40}Ca	96.982–96.880
^{42}Ca	0.656–0.640
^{43}Ca	0.146–0.131
^{44}Ca	2.130–2.057
^{46}Ca	0.0046–0.0031
^{48}Ca	0.200–0.179
V	
^{50}V	0.2502–0.2487
^{51}V	99.7513–99.7498
Cu	
^{63}Cu	69.24–68.98
^{65}Cu	31.02–30.76
Sr	
^{84}Sr	0.58–0.55
^{86}Sr	9.99–9.75
^{87}Sr	7.14–6.94
^{88}Sr	82.75–82.29
Ce	
^{136}Ce	0.186–0.185
^{138}Ce	0.254–0.251
^{140}Ce	88.449–88.446
^{142}Ce	11.114–11.114
Nd	
^{142}Nd	27.30–26.80
^{143}Nd	12.32–12.12
^{144}Nd	23.97–23.795
^{145}Nd	8.35–8.23
^{146}Nd	17.35–17.06
^{148}Nd	5.78–5.66
^{150}Nd	5.69–5.53
Hf	
^{174}Hf	0.1621–0.1619
^{176}Hf	5.271–5.206
^{177}Hf	18.606–18.593
^{178}Hf	27.297–27.278
^{179}Hf	13.630–13.619
^{180}Hf	35.100–35.076
Pb	
^{204}Pb	1.65–1.04
^{206}Pb	27.48–20.84
^{207}Pb	23.65–17.62
^{208}Pb	56.21–51.28
U	
^{234}U	0.0059–0.0050
^{235}U	0.7202–0.7198
^{238}U	99.2752–99.2739

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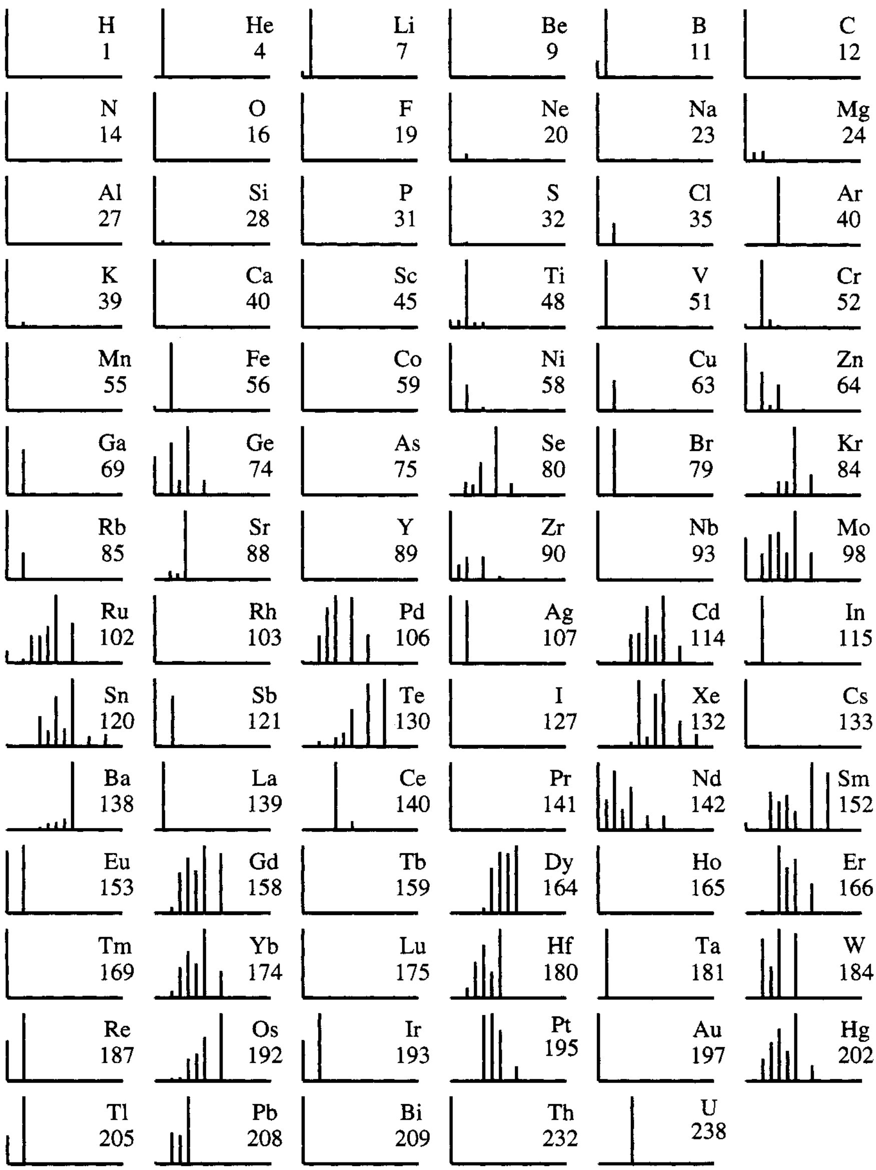
2.5.3
Isotope Patterns of Naturally Occurring Elements



The mass of the most abundant isotope is given under the symbol of the element. The lightest isotope is shown at the left end of the x axis.