

TABLE 13.4 Correlation of ¹H Chemical Shift with Environment












Type of proton	Formula	Chemical shift (δ)
Reference peak	(CH ₃) ₄ Si	0
Saturated primary	-CH ₃	0.7-1.3
Saturated secondary	-CH ₂ -	1.2-1.4
Saturated tertiary	 -H	1.4-1.7
Allylic primary	 -CH ₂	1.6-1.9
Methyl ketones	 -C(=O)CH ₃	2.1-2.4
Aromatic methyl	Ar-CH ₃	2.5-2.7
Alkyl chloride	Cl-  -H	3.0-4.0
Alkyl bromide	Br-  -H	2.5-4.0
Alkyl iodide	I-  -H	2.0-4.0
Alcohol, ether	-O-  -H	3.3-4.0
Alkynyl	-C≡C-H	2.5-2.7
Vinyllic	 -H	5.0-6.5
Aromatic	Ar-H	6.5-8.0
Aldehyde	 -H	9.7-10.0
Carboxylic acid	 -H	11.0-12.0
Alcohol	 -H	Extremely variable (2.5-5.0)

TABLE 13.5 Regions of the ¹H NMR Spectrum






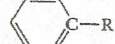




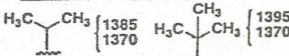
Region (δ)	Proton type	Comments
0-1.5	 -H	Protons on carbon next to saturated centers absorb in this region. Thus, the alkane portions of most organic molecules show complex absorption here.
1.5-2.5	 -H	Protons on carbon next to unsaturated centers (allylic, benzylic, next to carbonyl) show characteristic absorptions in this region, just downfield from other alkane resonance.
2.5-4.5	X-  -H	Protons on carbon next to electronegative atoms (halogen, O, N) are deshielded because of the electron-withdrawing ability of these atoms. Thus, the protons absorb in this midfield region.
4.5-6.5	 -H	Protons on double-bond carbons (vinylic protons) are strongly deshielded by the neighboring pi bond and therefore absorb in this characteristic downfield region.
6.5-8.0	 -H	Protons on aromatic rings (aryl protons) are strongly deshielded by the pi orbitals of the ring and absorb in this characteristic low-field range.

Table 13.7 ¹³C-NMR Chemical Shifts

Type of Carbon	Chemical Shift (δ)*	Type of Carbon	Chemical Shift (δ)*
RCH ₃	10-40	 -R	110-160
RCH ₂ R	15-55		160-180
R ₃ CH	20-60		165-180
RCH ₂ I	0-40		175-185
RCH ₂ Br	25-65		180-215
RCH ₂ Cl	35-80		
R ₂ COH	40-80		
R ₂ COR	40-80		
RC≡CR	65-85		
R ₂ C=CR ₂	100-150		

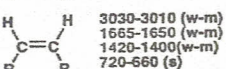
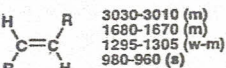
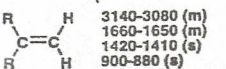
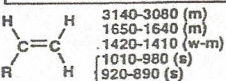
(s) = strong (m) = medium (w) = weak
br = broad v = very

Alkanes
 $sp^3 C-H$ 2960-2850 (s)
 $-CH_2-$ 1480-1445 (m-s)
 $[1350-1150; 1100-700]$
 $-CH_3$ 1380-1370 (m-s)
 $[1470-1430; 1100-700]$

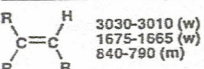


Alkenes
 $C=C$ 1660-1600 (vw-m)
 $C=C-H$ 3150-3000 (m)
 1000-650 (s)

C=C Substitution Pattern



Cyclic Alkenes
 $3C = 1641$ $5C = 1611$ $7C = 1650$
 $4C = 1566$ $6C = 1646$



Alkynes
 $C\equiv C-H$ 3320-3200 (s)
 700-600 (s)
 $C\equiv C$ 2250-2100 (w-m)

Nitrogen Functional Groups

$N-H$ 3500-3300 (w-s)
 $(RNH_2 = 2 \text{ bands}; R_2NH = 1 \text{ band})$

$1^\circ = 1640-1560$ (br, m)
 $C-N = 830-760$ (br, m)
 $2^\circ = 1510-1490$ (br, m)
 $C-N = 720-690$ (br, m)

$C-NR_2$ 1350-1000 (br, w-m)
 (aromatic) 1350-1250
 (aliphatic) 1250-1000

$R_2C=NR$ 1690-1640 (w-s)
 Imines [R = alkyl]; Oximes [R = OH]

(aliphatic) 1670-1650 (s)
 (aromatic) 1650-1645 (s)

$C\equiv N$ 2260-2220 (m-s)

$N\equiv N$ 2300-2100 (s-vs)

N_3 2250-2080 (vs)

NO_2 1600-1500 (s)
 1390-1300 (s)

Infrared Correlation Table

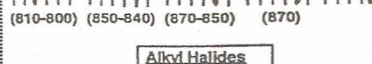
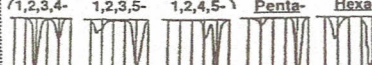
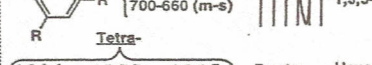
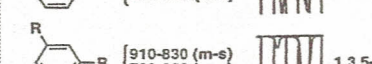
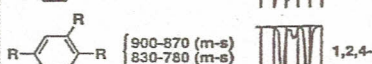
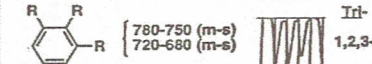
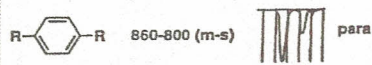
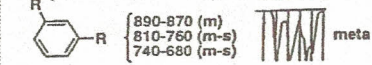
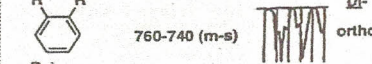
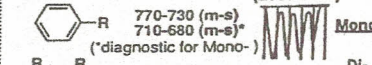
Compiled by Dr. Gary B. Fisher © 2001

Benzene
 $1610-1590$ (m-s) 3030 (m-s)
 $1510-1475$ (m-s) $900-690$ (m-s)

Substituted Benzenes: Overtone Regions
 $2000-1667$ (vw-m); $910-660$ (s);
 diagnostic; bands between $2000-1667$
 are often broadened, obscured, or absent

Substitution Pattern **Substitution Pattern**

(2000-1667)



Alkyl Halides
 $C-Cl$ 850-600 (s) H_2C-Cl 1300-1200 (s)
 $C-Br$ 680-590 (s) H_2C-Br 1250-1150 (s)
 $C-I$ 500-200 (s) H_2C-I 1200-1150 (s)

Alcohols and Ethers
 $O-H$ 3500-3200 (br, vs) (H-bonded)
 ["free" OH (non-H-bonded) = 3650-3600; sharp]

$C-O-H$ 1250-1000 (s)
 Free -OH $-C-O-$
 $1^\circ = -3640$ 1060-1040
 $2^\circ = -3630$ 1110-1090
 $3^\circ = -3620$ 1160-1140
 Phenol = -3610 1230-1210

$C-O-C$ 1300-1000 (s)
 $C-O-C$ (sp³) 1130-1110 $C-O-C$ 1260-1240
 950-815 $C-O-C$ 1050-1030
 850-750 $C-O-C$ 1225-1215
 1050-1030

$C-O-C$ 1300-1000 (s)
 $C-O-C$ (sp³) 1130-1110 $C-O-C$ 1260-1240
 950-815 $C-O-C$ 1050-1030
 850-750 $C-O-C$ 1225-1215
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$C-O-C$ 1300-1000 (s)
 $C-O-C$ (sp³) 1130-1110 $C-O-C$ 1260-1240
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 1050-1030

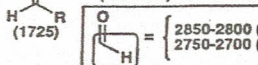
$C-O-C$ 1300-1000 (s)
 $C-O-C$ (sp³) 1130-1110 $C-O-C$ 1260-1240
 950-815 $C-O-C$ 1050-1030
 850-750 $C-O-C$ 1225-1215
 1050-1030

$C-O-C$ 1300-1000 (s)
 $C-O-C$ (sp³) 1130-1110 $C-O-C$ 1260-1240
 950-815 $C-O-C$ 1050-1030
 850-750 $C-O-C$ 1225-1215
 1050-1030

Carbonyl Compounds

General Range: 1830-1640 cm^{-1}
 All $C=O$ = (vs) $C=O$ overtones: 3500-3300 (w)
 (Base Value) α,β -unsaturated = -20 to -30

(aliphatic) 1720-1740
 (aromatic) 1685-1710



$1440-1160$ (m-s)
 (aliphatic) 1440-1320
 (aromatic) 1420-1350; 1320-1260; 1230-1160

(aliphatic) 1720-1710
 (aromatic) 1695-1685

$1300-1100$ (m-s)
 (aliphatic) 1220-1100
 (aromatic) 1300-1220

$1730-1700$
 $OH = 3400-2400$ (vbr, vs)
 $C-O = 1320-1210$ (m)

(X = Cl, Br)
 (aliphatic) 1810-1800
 (aromatic) 1770-1760

(aliphatic) 1740-1730
 (aromatic) 1720-1680
 (a-halo = +20)

1735 OR
 1735 OR

$1330-1000$ (vs)
 (≥ 2 sharp closely-spaced bands)

$1690-1640$ $1^\circ C-N = 1410-1390$ (s)
 $1125; 750-600$ (v.br) $2^\circ C-N = 1550-1500$ (s)

$1^\circ = 3450-3300$ (m-s)
 $3200-3150$
 $2^\circ = 3500-3100$ (m)
 ($1^\circ, 2^\circ$ often broadened)

$N-H$ bend: $1^\circ = 1640-1620$ (s)
 $2^\circ = 1550-1500$ (s)

$1830-1800$ (s)
 $1775-1740$ (s)

$1725-1715$ (Keto form)
 $1640-1610$ (br, s) (Enol form)
 [Enol form = H-bonding; $C=C$; 1600, (s)]

Sulfur-Oxygen Compounds

$1050-1000$ (s) $1370-1290$ (s) $1375-1350$ (s)
 $1170-1110$ (s) $1185-1165$ (s)

$S-O = 1000-750$ (s)

Boron Functional Groups

$B-H$ 2640-2200 (s) $B-C$ 1240-620 (s)
 $B-O$ 1380-1310 (vs) $B-F$ 1500-800 (s)
 $B-N$ 1550-1330 (vs) $B-Cl$ 1100-650 (s)

$2200-1540$ (m-s)
 (≥ 2 bands)

Pretsch, Clerc, Seibl, and Simon: Tables of Spectral Data for Structure Determination of Organic Compounds, Springer-Verlag, 1983; Pavia, Lampman, Kriz: Introduction to Spectroscopy, 2nd Ed., Saunders, 1996; Rappaport, Ed. Handbook of Tables for Organic Compound Identification, 3rd Ed., CRC Press, 1979, pp. 441-449; Conley: Infrared Spectroscopy, Allyn & Bacon, 1966