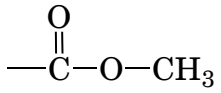
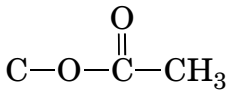
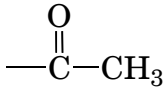
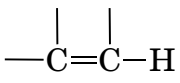
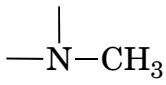
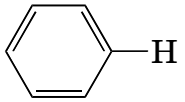
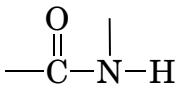
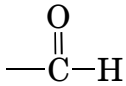
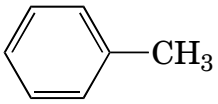
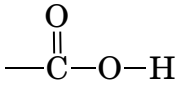
IR Absorption Bands of Functional Groups in Organic Compounds

Functional Group	Wavenumber (cm^{-1})	Comments
Alkane	**2850-3000**	**C–H stretch for sp^3 carbon (Strong)**
	1450-1470	C–H bend (Strong)
	1370-1380	**C–H methyl umbrella bend (Medium)**
	800-1200	C–C stretch (many medium bands)
	720-725	C–H bend (Medium)
Alkene	**3060-3140**	**C–H stretch for sp^2 carbon (Medium)**
	1620-1680	C=C stretch (Medium)
	900-1000	C–H bend (Strong)
Terminal alkyne (internal alkynes lack unique bands)	**3300-3320**	**C–H stretch for sp carbon (Medium)**
	2100-2140	C≡C stretch (medium)
	600-700	C–H bend (Strong)
Alcohol	**3200-3600**	**H–bonded O–H stretch (Broad strong band)**
	3600-3700	Free O–H stretch (sharp medium band, present only in dilute samples)
	1000-1200	C–O stretch (strong, higher ν for more substituents on carbon)
Ether	1050-1150	C–O stretch
Primary amine	3200-3400	N–H stretch (two medium bands)
Secondary amine	3200-3400	N–H stretch (single medium band)
Nitrile	2220-2280	N≡C stretch (medium)
Aldehyde	**1700-1720**	**C=O stretch (Strong)**
	2700-2850	Aldehyde C–H stretch, two medium bands
Ketone	**1680-1720**	**C=O stretch (Strong)**
Carboxylic acid	**1700-1720**	**C=O stretch (Strong)**
	3000	**O–H stretch** (very broad band, usually with a spike of sp^3 C–H stretch in the middle)
Ester	**1730-1750**	**C=O stretch (Strong)**
	1000-1300	C–O stretch
Amide	**1650-1690**	**C=O stretch (Strong)**
	3200-3400	N–H stretch (two bands for primary, one for secondary, none for tertiary amide)
Aromatic	3000-3150	C–H stretch (variable)
	1750-1950	C–H bending overtone region (usually several weak bands of similar strength)
	600-900	C–H bend (strong)
Nitro	**1550 and 1400**	"Walrus teeth" N–O stretch bands
Carbon dioxide	**2350**	Doublet (positive or negative, depending on variation in local concentration between baseline and sample measurement)

Predicting Chemical Shifts for ^{1}H-NMR Spectra
(adapted from Table 12.4, J.M. Hornback *Organic Chemistry*, 1998)

Type of Hydrogen	Chemical Shift (δ)	Type of Hydrogen	Chemical Shift (δ)
—C—CH_3	0.9	Br—CH_3	2.7
C=C—CH_3	1.6	Cl—CH_3	3.0
—C≡CH	1.8	—O—CH_3	3.3
	Variable (1-4)		3.7
—O—H	Variable (2-5)	O_2N—CH_3	4.1
	2.0	F—CH_3	4.2
	2.2		5.5-6.5
	2.2		7-8
I—CH_3	2.2		Variable (6-8)
N≡C—CH_3	2.2		10
	2.3		12

Procedure: Find the functional group near the proton of interest. Take the chemical shift listed and:
Add 0.3 if CH_2 instead of CH_3, or add 0.7 if CH instead of CH_3.
Add 0.3 for electronegative group or atom attached to the adjacent carbon.
When two electronegative groups are attached to the same carbon, both groups affect the hydrogens: add the indicated values from the table together, add the correction for the methylenyl or methinyl hydrogen, and subtract 0.9 from the total.

The value obtained by these calculations is a **prediction**, and may deviate from observed values by 1 ppm or more.

^{13}C NMR Chemical Shifts

Group	Chemical Shift	Group	Chemical Shift
Methyl	5-40	Ether	55-90
Methylene	15-55	Alkyne	60-90
Methine	25-60	Alkene	100-170
Alkyl chloride	40-50	Aromatic	90-160
Alkyl bromide	30-40	Alcohol	45-90
Alkyl iodide	5-15	Amine	10-70
Carbonyl (amide, carboxylic acid, ester)	150-185	Carbonyl (aldehyde, ketone)	175-220

Substituent Effects on Electrophilic Aromatic Substitution

Group	Effect	Regiochemistry
—NH_2 —NR_2 —OH —O^-	Strongly activating	*Ortho* / *para*
—O—R —S—R —NH—C(=O)—R —O—C(=O)—R	Moderately activating	*Ortho* / *para*
—R —Ar	Weakly activating	*Ortho* / *para*
—X	Weakly deactivating	*Ortho* / *para*
—C(=O)—H —C(=O)—R —C(=O)—OH —C(=O)—NH_2 —C(=O)—O—R	Moderately deactivating	*Meta*
—C≡N —SO_3H —CX_3 —NH_3^+ —NR_3^+ —NO_2	Strongly deactivating	*Meta*