

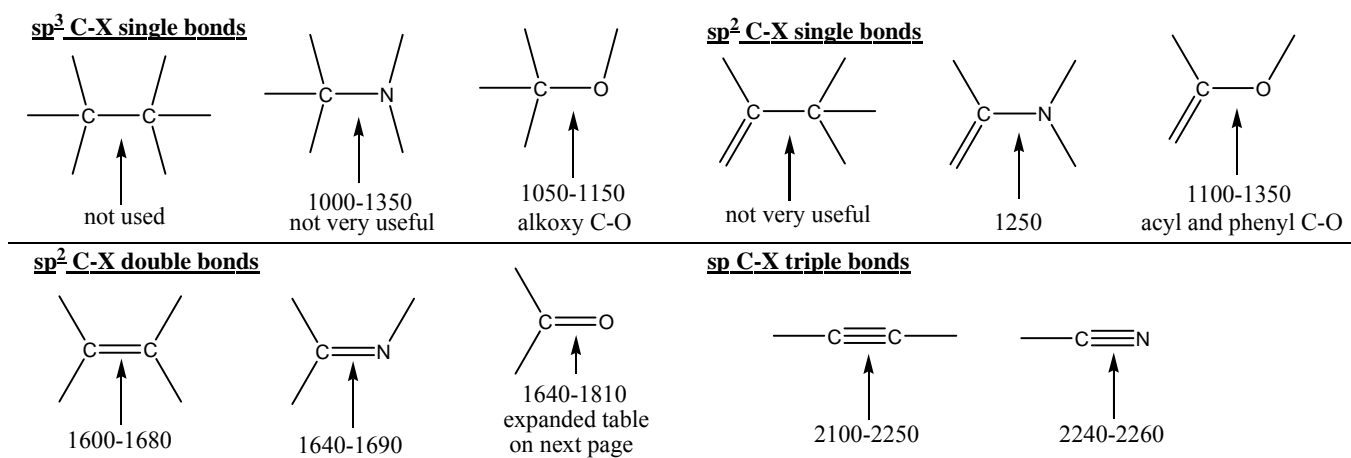
CHARACTERISTIC INFRARED ABSORPTION BANDS OF FUNCTIONAL GROUPS

Class of Compounds	Absorption, cm ⁻¹	Intensity	Assignment	Class of Compounds	Absorption, cm ⁻¹	Intensity	Assignment	
Alkanes and Alkyls	2850-3000	s	C-H stretch	Carboxylic Acids	2500-3500	s, broad	O-H stretch	
	1450-1470	s	C-H bend		R-C(O)-OH	1710-1715	s, broad	C=O stretch
	1370-1390	m	CH ₃ C-H bend		C=C-C(O)-OH or	1680-1710	s	C=O stretch
	1365 + 1395 (two bands)	m	-CH(CH ₃) ₂ or -(CH ₃) ₃ bend		Ar-C(O)-OH			
	715-725	w	-(CH ₂) _n bend		Esters	aliphatic 1160-1210 acetates ~1240 aromatic 1250-1310	s-vs	O=C-O-C stretch
Alkenes	3020-3140	w-m	=C-H stretch	R-C(O)-O-R	1735-1750	s	C=O stretch	
	1640-1670	vw-m	C=C stretch	C=C-C(O)-O-R or	1715-1730	s	C=O stretch	
	RCH=CH ₂	m + s	=C-H bend	Ar-C(O)-O-R				
	(two bands)			R-C(O)-O-Ar	1760-1790	s	C=O stretch	
	RR'C=CH ₂	s	=C-H bend	Acyl Chlorides				
	<i>cis</i> -RCH=CHR'	665-730	m-s, broad	=C-H bend	R-C(O)-Cl	1785-1815	s	C=O stretch
	<i>trans</i> -RCH=CHR'	960-980	s	=C-H bend	Ar-C(O)-Cl	1770-1800	s	C=O stretch
RCH=CR'R''	790-840	s	=C-H bend	Anhydrides				
Alkynes	R-C≡C-H	3265-3335	s, sharp	R-C(O)-O-C(O)-R	~1750 + ~1815	s,s	C=O symmetric	
		2100-2140	m	Ar-C(O)-O-C(O)-Ar	~1720 + ~1775	s,s	& asym. stretch	
		610-700	s, broad	(both two bands)				
	R-C≡C-R'	2190-2260	vw-w	C≡C stretch	Nitriles			
Alkyl halides	R-F	1000-1350	vs	R-C≡N	2240-2260	m-s	C≡N stretch	
	R-Cl	750-850	s	C=C-C≡N or	2220-2240	s	C≡N stretch	
	R-Br	500-680	s	Ar-C≡N				
	R-I	200-500	s	Amines				
				R-NH ₂	~3400 + ~3500 (two bands)	w	N-H symmetric & asym. stretch	
Alcohols	C=C-CH ₂ -OH	3300-3400	s, broad		1580-1650	w-m	N-H bend	
	R-CH ₂ -OH (1°) or	1035-1050	m-s	RR'N-H	3310-33350	w	N-H stretch	
	C=C-CH(R)-OH	1050-1085	m-s	Amides				
	RR'CH-OH (2°) or	1085-1125	m-s	R-C(O)-NH ₂	3200-3400 and 3400-3500 (two bands)	w-m	N-H symmetric & asym. stretch	
	C=C-CRR'-OH				1650-1690	s, broad	C=O stretch	
	RR'R''C-OH (3°)	1125-1205	m-s		1590-1655	m-s	N-H bend	
	Ar-O-H	1180-1260	m-s	R-C(O)-NH-R	3400-3500	w-m	N-H stretch	
Ethers	R-O-R'	1085-1150	s		1640-1690	s, broad	C=O stretch	
	Ar-O-R	1020-1075 and 1200-1275 (two band)	m-s	R-C(O)-NR'R''	1510-1560	m-s	N-H bend	
					1630-1680	m-s	C=O stretch	
Aldehydes	R-CH=O	2700-2725	m	Nitro Compounds				
	C=C-CH=O or	1720-1740	s	R-NO ₂	~1550 and ~1370	s	N-O symmetric & asym. stretch	
	Ar-CH=O	1685-1710	s	C=C-NO ₂ or	~1525 and ~1335	s	N-O symmetric & asym. stretch	
				Ar-NO ₂	(both two bands)			
Ketones	RR'C=O	1710-1720	s	Aromatic Compounds	3010-3100	m	Ar C-H stretch	
	C=C-C(O)-R	1665-1685	s		1450-1600	m-s	ring C=C stretch	
	Ar-C(O)-R	1675-1695	s		(two to four bands)	sharp		
	four member cyclic	1770-1780	s	monosubstituted	730-770 and 690-710 (two bands)	s	C-H bend	
	five member cyclic	1740-1755	s					
	six member cyclic	1710-1720	s	<i>o</i> -disubstituted	735-770	s	C-H bend	
				<i>m</i> -disubstituted	750-810 and 690-710	s	C-H bend	
				<i>p</i> -disubstituted	810-840	s	C-H bend	

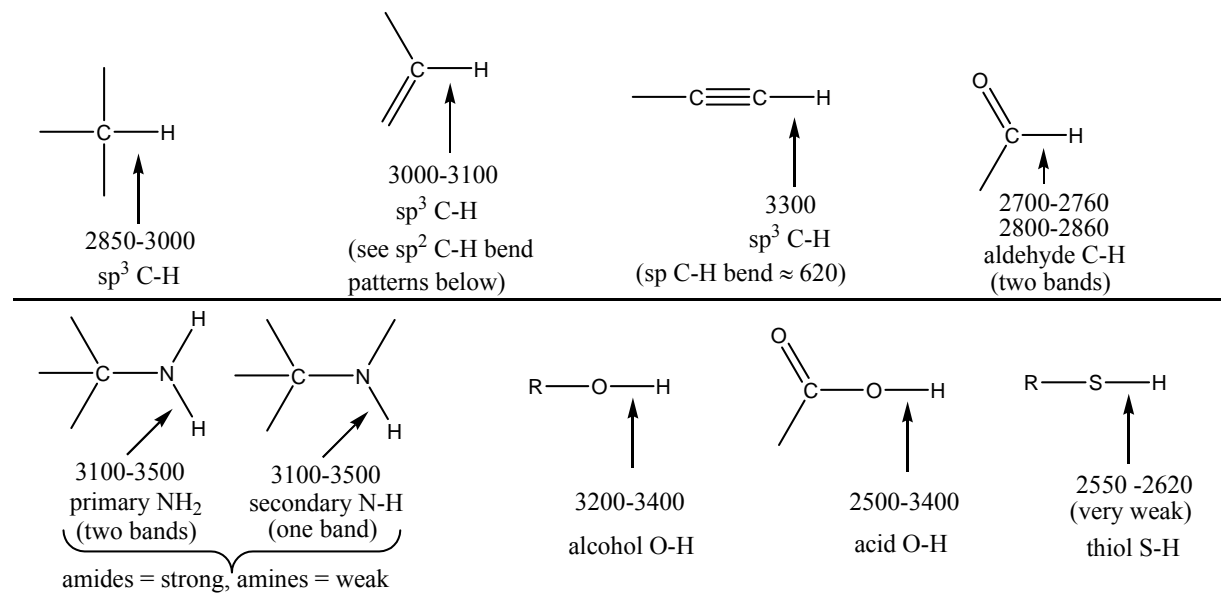
Intensity abbreviations: vw = very weak, w = weak, m = medium, s = strong, vs = very strong

Infrared Tables (short summary of common absorption frequencies)

The values given in the tables that follow are typical values. Specific bands may fall over a range of wavenumbers, cm^{-1} . Specific substituents may cause variations in absorption frequencies. Absorption intensities may be stronger or weaker than expected, often depending on dipole moments. Additional bands may confuse the interpretation. In very symmetrical compounds there may be fewer than the expected number of absorption bands (it is even possible that all bands of a functional group may disappear, i.e. a symmetrically substituted alkyne!). Infrared spectra are generally informative about what functional groups are present, but not always. The ^1H and ^{13}C NMR's are often just as informative about functional groups, and sometimes even more so in this regard. Information obtained from one spectroscopic technique should be verified or expanded by consulting the other spectroscopic techniques.

IR Summary - All numerical values in the tables below are given in wavenumbers, cm^{-1} **Bonds to Carbon (stretching wave numbers)**

Stronger dipoles produce more intense IR bands and weaker dipoles produce less intense IR bands (sometimes none).

Bonds to Hydrogen (stretching wave numbers)

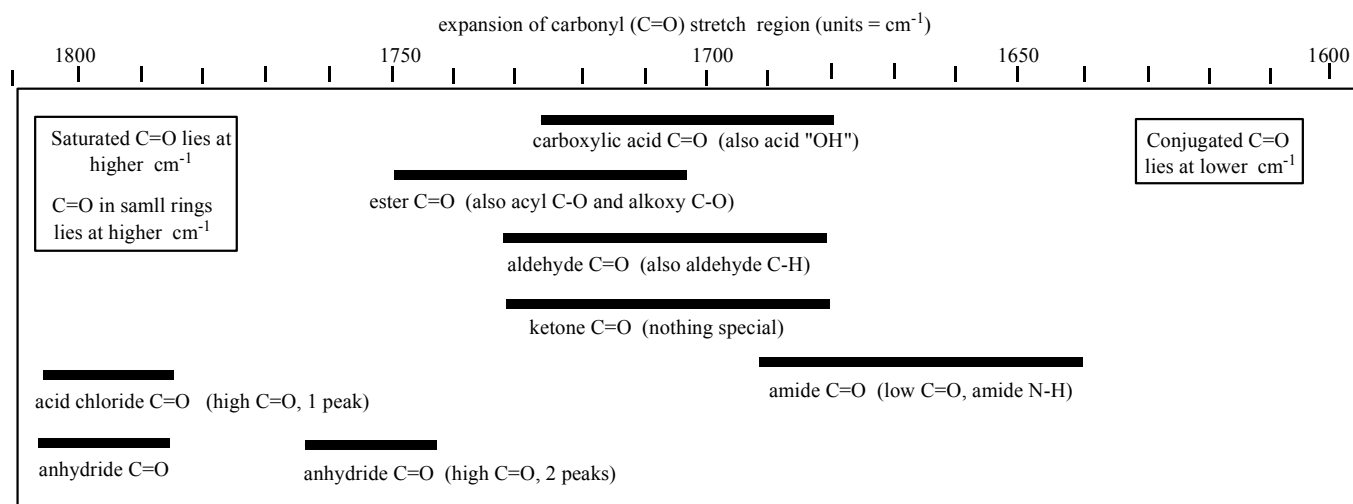
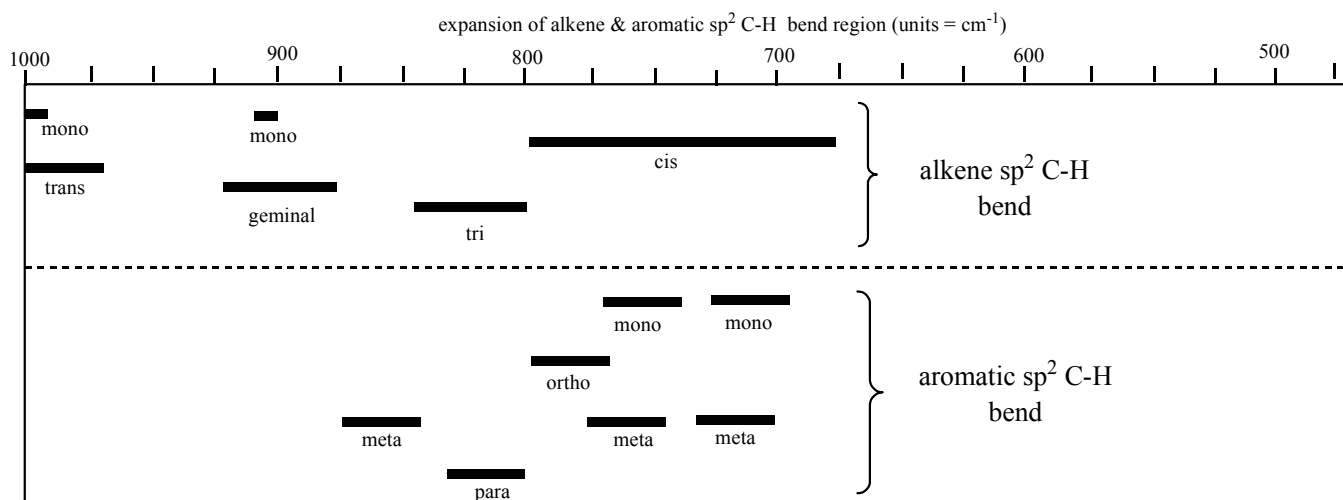
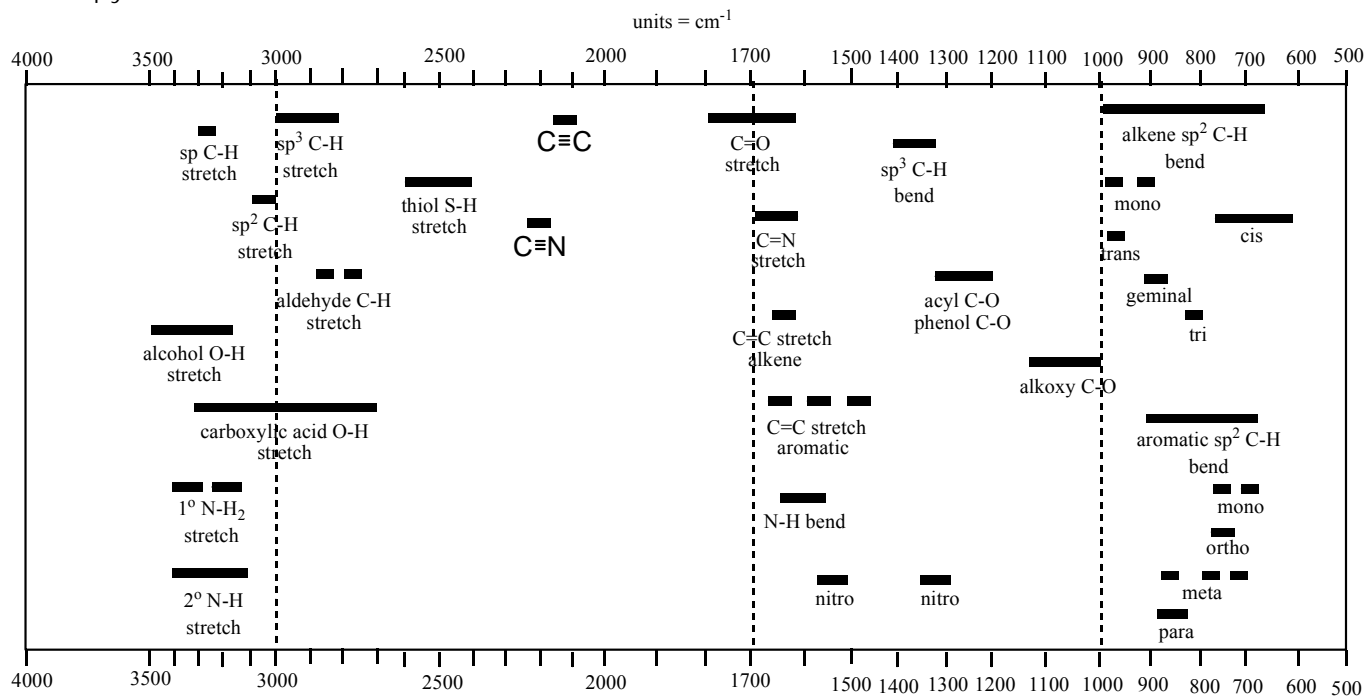
Carbonyl Highlights (stretching wave numbers)

Aldehydes	Ketones	Esters	Acids
saturated = 1725 conjugated = 1690 aromatic = 1700	saturated = 1715 conjugated = 1680 aromatic = 1690 6 atom ring = 1715 5 atom ring = 1745 4 atom ring = 1780 3 atom ring = 1850	saturated = 1735 conjugated = 1720 aromatic = 1720 6 atom ring = 1735 5 atom ring = 1775 4 atom ring = 1840 RCOOAr = 1780	saturated = 1715 conjugated = 1690 aromatic = 1690
Amides	Anhydrides	Acid Chlorides	nitro
saturated = 1650 conjugated = 1660 aromatic = 1660 6 atom ring = 1670 5 atom ring = 1700 4 atom ring = 1745 3 atom ring = 1850	saturated = 1760, 1820 conjugated = 1725, 1785 aromatic = 1725, 1785 6 atom ring = 1750, 1800 5 atom ring = 1785, 1865	saturated = 1800 conjugated = 1770 aromatic = 1770	asymmetric = 1500-1600 symmetric = 1300-1390
Very often there is a very weak C=O overtone at approximately $2 \times \bar{\nu}$ ($\approx 3400 \text{ cm}^{-1}$). Sometimes this is mistaken for an OH or NH peak.			









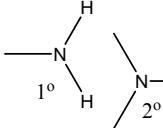
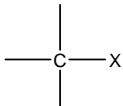
sp² C-H bend patterns for alkenes**sp² C-H bend patterns for aromatics**

alkene substitution pattern	descriptive alkene term	absorption frequencies (cm ⁻¹) due to sp ² CH bend	aromatic substitution pattern	descriptive aromatic term	absorption frequencies (cm ⁻¹) due to sp ² CH bend
	monosubstituted alkene	985-1000 900-920		monosubstituted aromatic	690-710 730-770
	cis disubstituted alkene	675-730 (broad)		ortho disubstituted aromatic	735-770
	trans disubstituted alkene	960-990		meta disubstituted aromatic	680-725 750-810 880-900 (sometimes)
	geminal disubstituted alkene	880-900		para disubstituted aromatic	790-840
	trisubstituted alkene	790-840			
	tetrasubstituted alkene	none			

Aromatic compounds have characteristic weak overtone bands that show up between 1650-2000 cm⁻¹. Some books provide pictures for comparison (not here). A strong C=O peak will cover up most of this region.



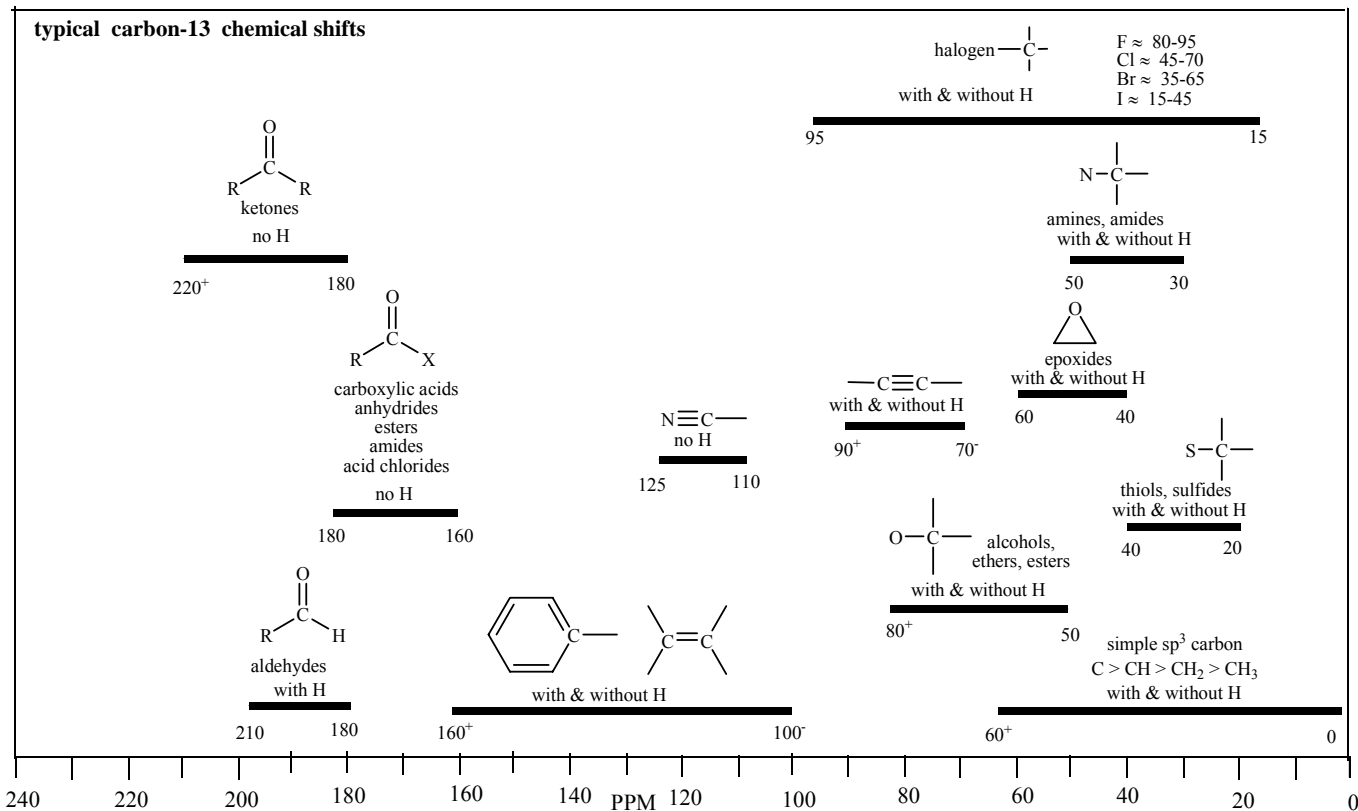
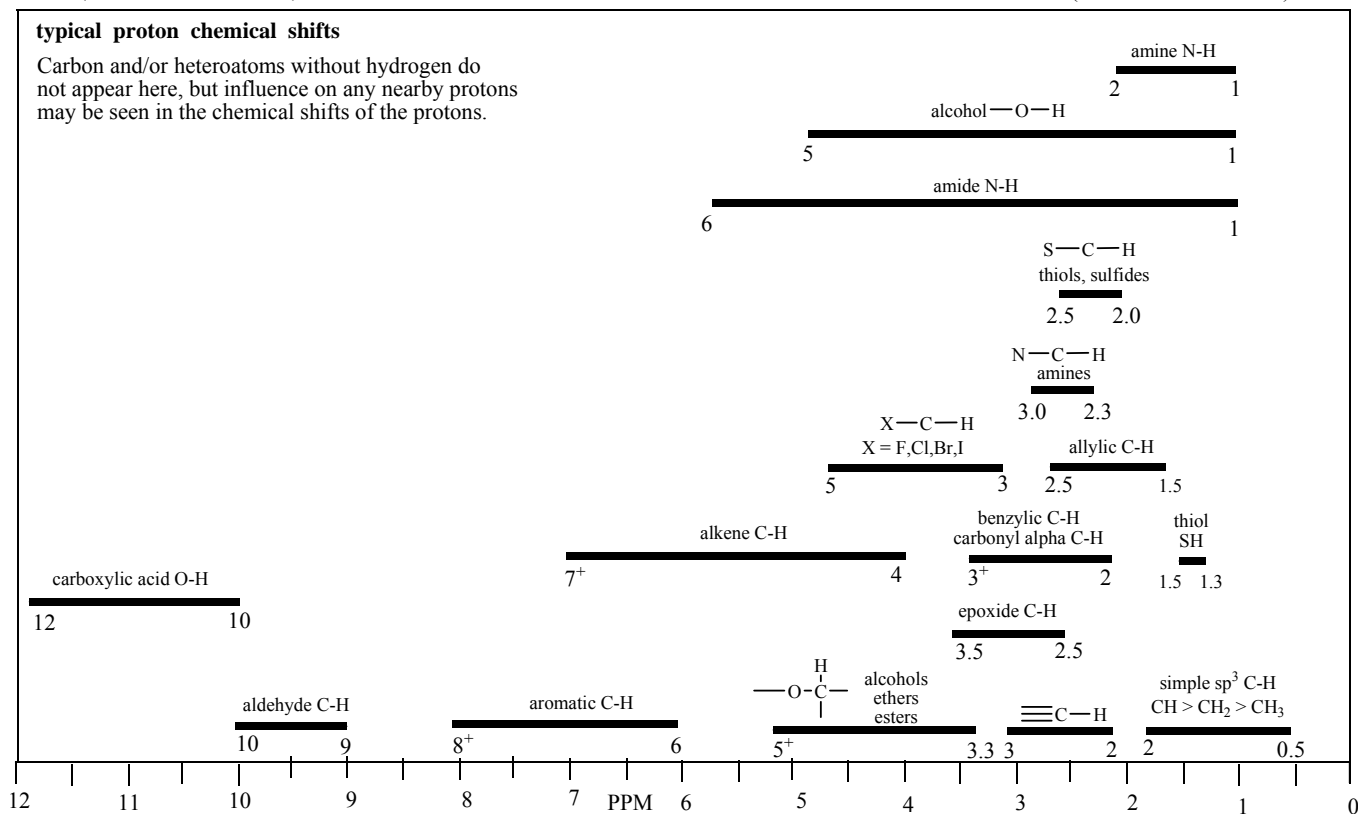
IR Flowchart to determine functional groups in a compound (all values in cm^{-1}).**IR Spectrum**

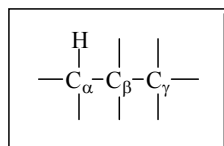
IR Spectrum		has C=O band (1650-1800 cm^{-1}) very strong	does not have C=O band						
<p>aldehydes</p>  <p>1725-1740 (saturated) 1660-1700 (unsaturated)</p> <p>2860-2800 ← sometimes lost 2760-2700 in sp^3 CH peaks (both weak)</p> <p>aldehyde C-H</p>		<p>alkanes</p> <table border="1"> <tr><td>sp^3 C-H stretch</td><td>2850-3000</td></tr> <tr><td>sp^3 C-H bend</td><td>1460 & 1380</td></tr> <tr><td>C—C</td><td>not useful</td></tr> </table>		sp^3 C-H stretch	2850-3000	sp^3 C-H bend	1460 & 1380	C—C	not useful
sp^3 C-H stretch	2850-3000								
sp^3 C-H bend	1460 & 1380								
C—C	not useful								
<p>ketones</p>  <p>1710-1720 (saturated) 1680-1700 (unsaturated) 1715-1810 (rings: higher in small rings)</p>		<p>nitriles</p> <p>$\text{C}\equiv\text{N}$</p> <p>≈ 2250 sharp, stronger than alkynes, a little lower when conjugated</p>							
<p>esters - rule of 3</p>  <p>1735-1750 (saturated) 1715-1740 (unsaturated) 1735-1820 (higher in small rings)</p> <p>acyl C—O 1150-1350 (acyl, strong)</p> <p>alkoxy C—O (1000-1150, alkoxy, medium)</p>		<p>alkynes</p> <p>$\text{C}\equiv\text{C}$</p> <p>2150 (variable intensity)</p> <p>not present or weak when symmetrically substituted, a little lower when conjugated</p>							
<p>acids</p>  <p>1700-1730 (saturated) 1715-1740 (unsaturated) 1680-1700 (higher in small rings)</p> <p>acyl C—O 1210-1320 (acyl, strong)</p> <p>acid O—H 2400-3400, very broad (overlaps C-H stretch)</p>		<p>alkenes</p> <p>sp^2 C-H stretch 3000-3100</p> <p>sp^2 C-H bend 650-1000 (see table for spectral patterns)</p> <p>C=C 1600-1660 weak or not present</p>							
<p>amides</p>  <p>1630-1680 (saturated) 1745 (in 4 atom ring)</p> <p>1° 3350 & 3180, two bands for 1° amides, one band for 2° amides, stronger than in amines, extra overtone sometimes at 3100</p> <p>2°</p> <p>N—H N-H bend, 1550-1640, stronger in amides than amines</p>		<p>aromatics</p> <p>sp^2 C-H stretch 3050-3150</p> <p>sp^2 C-H bend 690-900 (see table), overtone patterns between 1660-2000</p> <p>C=C 1600 & 1480 can be weak</p>							
<p>acid chlorides</p>  <p>1800 (saturated) 1770 (unsaturated)</p> <p>Inductive pull of Cl increases the electron density between C and O.</p>		<p>alcohols</p> <p>alcohol O—H 3600-3500</p> <p>alkoxy C—O 1000-1260 ($3^\circ > 2^\circ > 1^\circ$)</p>							
<p>anhydrides</p>  <p>1760 & 1820 (saturated) 1725-1785 (unsaturated) two strong bands</p> <p>acyl C—O 1150-1350 (acyl, strong)</p>		<p>thiols</p> <p>thiol S—H ≈ 2550 (weak) (easy to overlook)</p>							
<p>nitro compounds</p>  <p>1500-1600, asymmetric (strong) 1300-1390, symmetric (medium)</p>		<p>amines</p>  <p>1° 3300 - 3500, two bands for 1° amines, one band for 2° amines, weaker than in amides,</p> <p>2°</p> <p>N—H N-H bend, 1550-1640, stronger in amides than amines</p> <p>N—C 1000-1350 (uncertain)</p>							
<p>carbon-halogen bonds</p>  <p>usually not very useful</p> <p>X = F, Cl, Br, I</p>		<p>ethers</p> <p>alkoxy C—O 1120 (aliphatic) 1040 & 1250 (aromatic)</p>							
<p>All IR values are approximate and have a range of possibilities depending on the molecular environment in which the functional group resides. Resonance often modifies a peak's position because of electron delocalization (C=O lower, acyl C-O higher, etc.). IR peaks are not 100% reliable. Peaks tend to be stronger (more intense) when there is a large dipole associated with a vibration in the functional group and weaker in less polar bonds (to the point of disappearing in some completely symmetrical bonds).</p>		<p>Alkene sp^2 C-H bending patterns</p> <p>monosubstituted (985-1000, 900-920) geminal disubstituted (960-990) cis disubstituted (675-730) trans disubstituted (880-900) trisubstituted (790-840) tetrasubstituted (none, no sp^2 C-H)</p>							
<p>Aromatic sp^2 C-H bending patterns</p> <p>monosubstituted (730-770, 690-710) ortho disubstituted (735-770) meta disubstituted (880-900, sometimes, 750-810, 680-725) para disubstituted (790-840)</p> <p>There are also weak overtone bands between 1660 and 2000, but are not shown here. You can consult pictures of typical patterns in other reference books. If there is a strong C=O band, they may be partially covered up.</p>									

deshielding side = less electron rich
(inductive & resonance)

Typical ^1H and ^{13}C NMR chemical shift values.

shielding side = more electron rich
(inductive & resonance)



Calculation of chemical shifts for protons at sp^3 carbons

Estimation of sp^3 C-H chemical shifts with multiple substituent parameters for protons within 3 C's of consideration.

α = directly attached substituent, use these values when the hydrogen and substituent are attached to the same carbon

β = once removed substituent, use these values when the hydrogen and substituent are on adjacent (vicinal) carbons

γ = twice removed substituent, use these values when the hydrogen and substituent have a 1,3 substitution pattern

X = substituent	α	β	γ
R- (alkyl)	0.0	0.0	0.0
R ₂ C=CR- (alkenyl)	0.8	0.2	0.1
RCC- (alkynyl)	0.9	0.3	0.1
Ar- (aromatic)	1.4	0.4	0.1
F- (fluoro)	3.2	0.5	0.2
Cl- (chloro)	2.2	0.5	0.2
Br- (bromo)	2.1	0.7	0.2
I- (iodo)	2.0	0.9	0.1
HO- (alcohol)	2.3	0.3	0.1
RO- (ether)	2.1	0.3	0.1
epoxide	1.5	0.4	0.1
R ₂ C=CRO- (alkenyl ether)	2.5	0.4	0.2
ArO- (aromatic ether)	2.8	0.5	0.3
RCO ₂ - (ester, oxygen side)	2.8	0.5	0.1
ArCO ₂ - (aromatic ester, oxygen side)	3.1	0.5	0.2
ArSO ₃ - (aromatic sulfonate, oxygen)	2.8	0.4	0.0
H ₂ N- (amine nitrogen)	1.5	0.2	0.1
RCONH- (amide nitrogen)	2.1	0.3	0.1
O ₂ N- (nitro)	3.2	0.8	0.1
HS- (thiol, sulfur)	1.3	0.4	0.1
RS- (sulfide, sulfur)	1.3	0.4	0.1
OHC- (aldehyde)	1.1	0.4	0.1
RCO- (ketone)	1.2	0.3	0.0
ArCO- (aromatic ketone)	1.7	0.3	0.1
HO ₂ C- (carboxylic acid)	1.1	0.3	0.1
RO ₂ C- (ester, carbon side)	1.1	0.3	0.1
H ₂ NOC- (amide, carbon side)	1.0	0.3	0.1
ClOC- (acid chloride)	1.8	0.4	0.1
NC- (nitrile)	1.1	0.4	0.2
RSO- (sulfoxide)	1.6	0.5	0.3
RSO ₂ - (sulfone)	1.8	0.5	0.3

Starting value and equations for CH₃'s

$$\delta \text{CH}_3 = 0.9 + \alpha \quad \text{H}_3\text{C}-\alpha$$

$$\delta \text{CH}_3 = 0.9 + \sum(\beta + \gamma) \quad \text{H}_3\text{C}-\text{C}_\beta-\text{C}_\gamma$$

Σ is the summation symbol for all substituents considered

Starting value and equation for CH₂'s

In a similar manner we can calculate chemical shifts for methylenes (CH₂) using the following formula

$$\delta \text{CH}_2 = 1.2 + \sum(\alpha + \beta + \gamma) \quad \text{H}-\text{C}_\alpha-\text{C}_\beta-\text{C}_\gamma$$

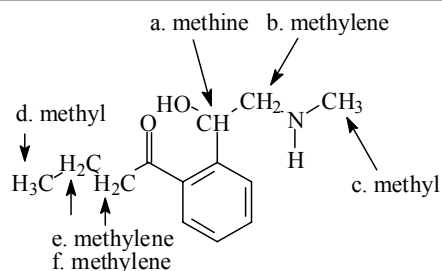
Σ is the summation symbol for all substituents considered

Starting value and equation for CH's

In a similar manner we can calculate chemical shifts for methines (CH) using the following formula

$$\delta \text{CH} = 1.5 + \sum(\alpha + \beta + \gamma) \quad \text{H}-\text{C}_\alpha-\text{C}_\beta-\text{C}_\gamma$$

Σ is the summation symbol for all substituents considered



$$\begin{aligned} \text{a. methine} &= 1.5 + (1.4)_\alpha + (2.3)_\alpha + (0.2)_\beta = 5.4 \text{ ppm} \\ \text{actual} &= 5.2 \end{aligned}$$

$$\begin{aligned} \text{b. methylene} &= 1.2 + (1.5)_\alpha + (0.4)_\beta + (0.3)_\beta = 3.4 \text{ ppm} \\ \text{actual} &= 3.0 \text{ and } 3.2 \end{aligned}$$

$$\begin{aligned} \text{c. methyl} &= 0.9 + (1.5)_\alpha = 2.4 \text{ ppm} \\ \text{actual} &= 2.6 \end{aligned}$$

$$\begin{aligned} \text{d. methyl} &= 0.9 + (0.1)_\alpha = 1.0 \text{ ppm} \\ \text{actual} &= 1.0 \end{aligned}$$

$$\begin{aligned} \text{e. methylene} &= 1.2 + (0.3)_\alpha = 1.5 \text{ ppm} \\ \text{actual} &= 1.7 \end{aligned}$$

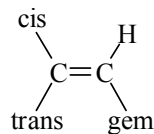
$$\begin{aligned} \text{f. methylene} &= 1.2 + (1.7)_\alpha = 2.9 \text{ ppm} \\ \text{actual} &= 2.9 \end{aligned}$$

Calculations are generally close to actual chemical shifts for a single substituent, but are less reliable as the number of substituent factors goes up. Multiple substituent factors tend to overestimate an actual chemical shift.

Estimated chemical shifts for protons at alkene sp^2 carbons

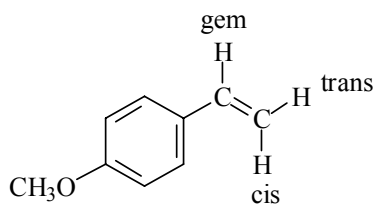
Substituent	α_{geminal}	α_{cis}	α_{trans}
H- Hydrogen	0.0	0.0	0.0
R- Alkyl	0.5	-0.2	-0.3
$C_6H_5CH_2$ - Benzyl	0.7	-0.2	-0.2
X- CH_2 - Halomethyl	0.7	0.1	0.0
(H)/ $ROCH_2$ - alkoxymethyl	0.6	0.0	0.0
(H) $_2$ / R_2NCH_2 - aminomethyl	0.6	-0.1	-0.1
$RCOCH_2$ - α -keto	0.7	-0.1	-0.1
$NCCH_2$ - α -cyano	0.7	-0.1	-0.1
$R_2C=CR$ - Alkenyl	1.2	0.0	0.0
C_6H_5 - Phenyl	1.4	0.4	-0.1
F- Fluoro	1.5	-0.4	-1.0
Cl- Chloro	1.1	0.2	0.1
Br- Bromo	1.1	0.4	0.6
I- Iodo	1.1	0.8	0.9
RO - alkoxy (ether)	1.2	-1.1	-1.2
RCO_2 - O-ester	2.1	-0.4	-0.6
(H) $_2$ / R_2N - N-amino	0.8	-1.3	-1.2
$RCONH$ - N-amide	2.1	-0.6	-0.7
O_2N - Nitro	1.9	1.3	0.6
RS - Thiol	1.1	-0.3	-0.1
OHC - Aldehyde	1.0	1.0	1.2
ROC - Ketone	1.1	0.9	0.7
HO_2C - C-acid	0.8	1.0	0.3
RO_2C - C-ester	0.8	1.0	0.5
H_2NOC - C-amide	1.30	1.0	0.5
NC - Nitrile	0.3	0.8	0.6

Substitution relative to calculated "H"



$$\delta(\text{ppm}) = 5.2 + \alpha_{\text{gem}} + \alpha_{\text{cis}} + \alpha_{\text{trans}}$$

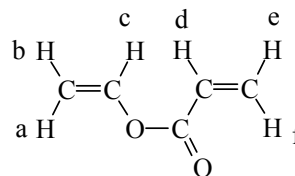
Example Calculation



$$\begin{aligned} \delta_{\text{gem}} &= 5.2 + 1.4 = 6.6 \\ \text{actual} &= 6.6 \end{aligned}$$

$$\begin{aligned} \delta_{\text{trans}} &= 5.2 - 0.1 = 5.1 \\ \text{actual} &= 5.1 \end{aligned}$$

$$\begin{aligned} \delta_{\text{cis}} &= 5.2 + 0.4 = 5.7 \\ \text{actual} &= 5.6 \end{aligned}$$



$$\begin{aligned} \delta_a &= 5.2 + (-0.4) = 4.8 \\ \text{actual} &= 4.9 \quad (J = 14, 1.6 \text{ Hz}) \end{aligned}$$

$$\begin{aligned} \delta_b &= 5.2 + (-0.6) = 4.6 \\ \text{actual} &= 4.6 \quad (J = 6, 1.6 \text{ Hz}) \end{aligned}$$

$$\begin{aligned} \delta_c &= 5.2 + 2.1 = 7.3 \\ \text{actual} &= 7.4 \quad (J = 14, 6 \text{ Hz}) \end{aligned}$$

$$\begin{aligned} \delta_d &= 5.2 + 0.8 = 6.0 \\ \text{actual} &= 6.2 \quad (J = 18, 11 \text{ Hz}) \end{aligned}$$

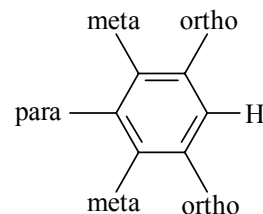
$$\begin{aligned} \delta_e &= 5.2 + 0.5 = 5.7 \\ \text{actual} &= 5.8 \quad (J = 11, 1.4 \text{ Hz}) \end{aligned}$$

$$\begin{aligned} \delta_f &= 5.2 + 1.0 = 6.2 \\ \text{actual} &= 6.4 \quad (J = 18, 1.4 \text{ Hz}) \end{aligned}$$

Estimated chemical shifts for protons at aromatic sp^2 carbons

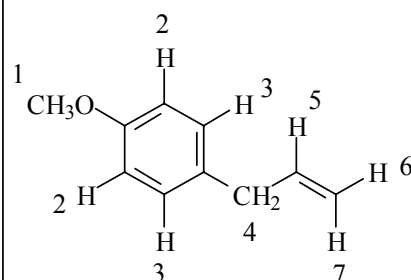
Substituent	α ortho	α meta	α para
H- Hydrogen	0.0	0.0	0.0
CH ₃ - Methyl	-0.2	-0.1	-0.2
ClCH ₂ - Chloromethyl	0.0	0.0	0.0
Cl ₃ C- Halomethyl	0.6	0.1	0.1
HOCH ₂ - Hydroxymethyl	-0.1	-0.1	-0.1
R ₂ C=CR- Alkenyl	0.1	0.0	-0.1
C ₆ H ₅ - Phenyl	1.4	0.4	-0.1
F- Fluoro	-0.3	0.0	-0.2
Cl- Chloro	0.0	0.0	-0.1
Br- Bromo	0.2	-0.1	0.0
I- Iodo	0.4	-0.2	0.9
HO- Hydroxy	-0.6	-0.1	-0.5
RO- Alkoxy	-0.5	-0.1	-0.4
RCO ₂ - O-ester	-0.3	0.0	-0.1
(H) ₂ /R ₂ N- N-amino	-0.8	-0.2	-0.7
RCONH- N-amide	0.1	-0.1	-0.3
O ₂ N- Nitro	1.0	0.3	0.4
RS- thiol/sulfide	-0.1	-0.1	-0.2
OHC- Aldehyde	0.6	0.2	0.3
ROC- Ketone	0.6	0.1	0.2
HO ₂ C- C-acid	0.9	0.2	0.3
RO ₂ C- C-ester	0.7	0.1	0.2
H ₂ NOC- C-amide	0.6	0.1	0.2
NC- Nitrile	0.4	0.2	0.3

Substitution relative to calculated "H"



$$\delta(\text{ppm}) = 7.3 + \alpha_{\text{ortho}} + \alpha_{\text{meta}} + \alpha_{\text{para}}$$

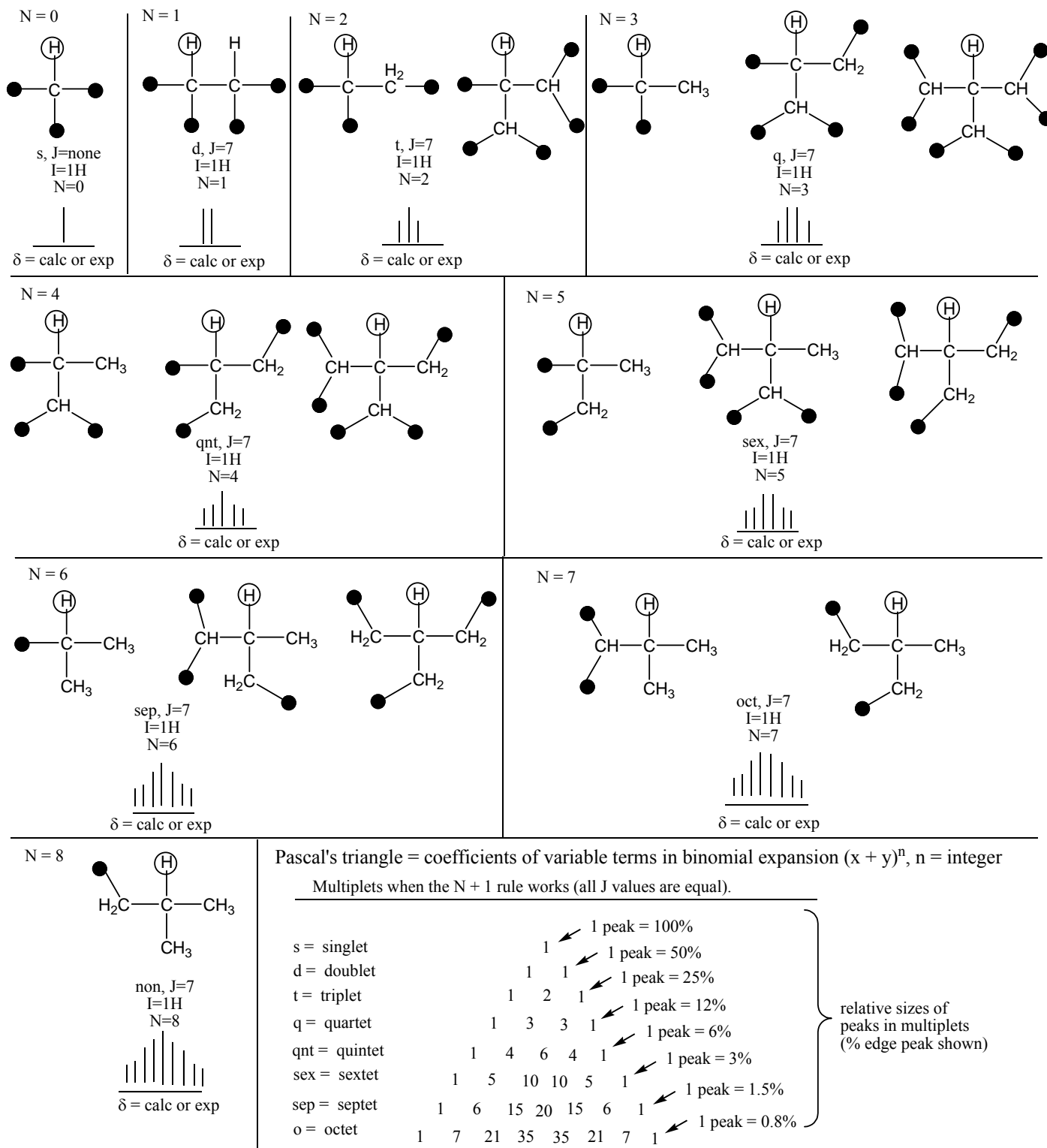
Example Calculation



- $\delta(\text{CH}_3) = 0.9 + 2.8 = 3.7$
actual = 3.8
- $\delta(2) = 7.3 + (-0.5)_{\text{ortho}} + (-0.1)_{\text{para}} = 6.7$
actual = 6.8
- $\delta(3) = 7.3 + (-0.2)_{\text{ortho}} + (-0.4)_{\text{para}} = 6.7$
actual = 7.1
- $\delta(\text{CH}_2) = 1.2 + (0.8)\alpha + (1.4)\alpha = 3.4$
actual = 3.3
- $\delta(5) = 5.2 + (0.7)_{\text{gem}} = 5.9$
actual = 5.9
- $\delta(6) = 5.2 + (-0.2)_{\text{trans}} = 5.0$
actual = 5.1
- $\delta(7) = 5.2 + (-0.2)_{\text{cis}} = 5.0$
actual = 5.1

Splitting patterns when the N+1 rule works (common, but not always true)


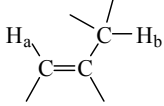
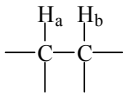
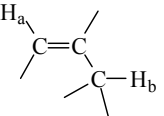
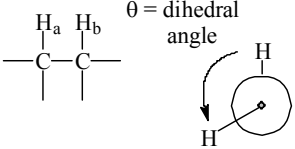
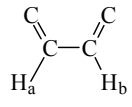
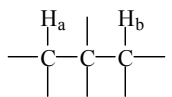
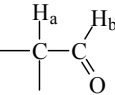
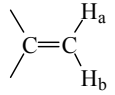
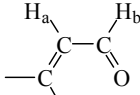
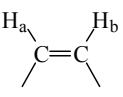
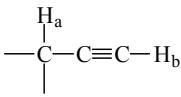
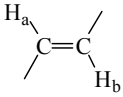
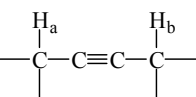
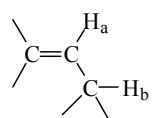
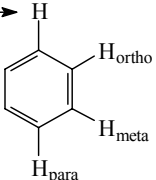
● = group without any coupled proton(s)



Combinations of these are possible.

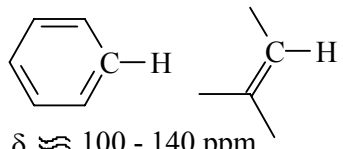
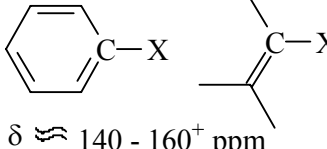
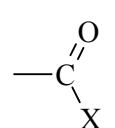
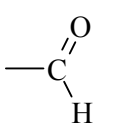
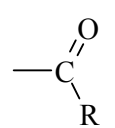
dd = doublet of doublets; ddd = doublet of doublet of doublets; dddd = doublet of doublet of doublet of doublets; dt = doublet of triplets; td = triplet of doublets; etc.

Typical Coupling Constants

	<u>Range</u>	<u>Typical</u>		<u>Range</u>	<u>Typical</u>
 <p>geminal protons - can have different chemical shifts and split one another if they are diastereotopic</p>	0-30 Hz	14 Hz	 <p>cis / allylic coupling, notice through 4 bonds</p>	0-3 Hz	1 Hz
 <p>vicinal protons are on adjacent atoms, when freely rotating coupling averages out to about 7 Hz</p>	6-8 Hz	7 Hz	 <p>trans / allylic coupling, notice through 4 bonds</p>	0-3 Hz	1 Hz
 <p>θ = dihedral angle</p> <p>depends on dihedral angle, see plot of Karplus equation</p>	0-12 Hz	7 Hz	 <p>sp² vicinal coupling (different π bonds)</p>	9-13 Hz	10 Hz
 <p>protons rarely couple through 4 chemical bonds unless in a special, rigid shapes (i.e. W coupling)</p>	0-1 Hz	0 Hz	 <p>sp³ vicinal aldehyde coupling</p>	1-3 Hz	2 Hz
 <p>sp² geminal coupling</p>	0-3 Hz	2 Hz	 <p>sp² vicinal aldehyde coupling</p>	5-8 Hz	6 Hz
 <p>sp² cis (acyclic) coupling (always smaller than the trans isomer)</p>	5-11 Hz	10 Hz	 <p>sp / propargylic coupling notice through 4 bonds</p>	2-3 Hz	2 Hz
 <p>sp² trans coupling (always larger than the cis isomer)</p>	11-19 Hz	17 Hz	 <p>bis-propargylic coupling notice through 5 bonds</p>	2-3 Hz	3 Hz
 <p>sp² / sp³ vicinal coupling</p>	4-10 Hz	7 Hz	<p>ortho, meta and para coupling to this proton</p>  <p>ortho H_{ortho} meta H_{meta} para H_{para}</p>	<p>ortho 6-10 Hz</p> <p>meta 2-3 Hz</p> <p>para 0-1 Hz</p>	<p>9 Hz</p> <p>2 Hz</p> <p>0 Hz</p>

When J values are less than 1 Hz, it is often difficult to resolve them and a peak may merely appear wider and shorter.

Similar chemical shift information presented in a different format. Remember, proton decoupled carbons appear as singlets. When carbons are coupled to their hydrogens, carbons follow the N+1 rule. Methyls = q, methylenes = t, methines = d, and carbons without hydrogen appear as singlets = s. DEPT provides the same information. Carbon chemical shifts are spread out over a larger range than proton chemical shifts (they are more dispersed), so it is less likely that two different carbon shifts will fall on top of one another. The relative positions of various types of proton and carbon shifts have many parallel trends (shielded protons tend to be on shielded carbons, etc.)

Simple alkane carbons	CH_3- $d \approx 0 - 30 \text{ ppm}$ (q)	CH_2- $d \approx 20 - 40 \text{ ppm}$ (t)	$-\text{CH}-$ $d \approx 30 - 50 \text{ ppm}$ (d)	$-\text{C}-$ $d \approx 30 - 60 \text{ ppm}$ (s)
sp^3 carbon next to oxygen	CH_3-O $d \approx 50 - 60 \text{ ppm}$ (q)	CH_2-O $d \approx 55 - 80 \text{ ppm}$ (t)	$-\text{CH}-\text{O}$ $d \approx 60 - 80 \text{ ppm}$ (d)	$-\text{C}-\text{O}$ $d \approx 70 - 90 \text{ ppm}$ (s)
sp^3 carbon next to nitrogen	CH_3-N $d \approx 10 - 50 \text{ ppm}$ (q)	CH_2-N $d \approx 35 - 55 \text{ ppm}$ (t)	$-\text{CH}-\text{N}$ $d \approx 50 - 70 \text{ ppm}$ (d)	$-\text{C}-\text{N}$ $d \approx 50 - 70 \text{ ppm}$ (s)
sp^3 carbon next to bromine or chlorine (X = Cl, Br)		CH_2-X $d \approx 25 - 50 \text{ ppm}$ (t)	$-\text{CH}-\text{X}$ $d \approx 60 - 80 \text{ ppm}$ (d)	$-\text{C}-\text{X}$ $d \approx 60 - 80 \text{ ppm}$ (s)
sp carbon (alkynes)	$-\text{C}\equiv\text{C}-$ $\delta \approx 70 - 90 \text{ ppm}$		sp carbon (nitriles)	$-\text{C}\equiv\text{N}$ $\delta \approx 110 - 125 \text{ ppm}$
sp^2 carbon (alkenes and aromatics)	 $\delta \approx 100 - 140 \text{ ppm}$ simple sp^2 carbon resonance donation moves δ lower, resonance withdrawal moves δ higher	 $\delta \approx 140 - 160^+ \text{ ppm}$ sp^2 carbon attached to an electronegative atom (X = oxygen, nitrogen, halogen) or C_β carbon conjugated with a carbonyl group		
 $\delta \approx 160 - 180 \text{ ppm}$ carboxyl carbons (acids, esters, amides) (s)	 $\delta \approx 180 - 210 \text{ ppm}$ aldehyde carbons, lower values when conjugated (d)	 $\delta \approx 180 - 220 \text{ ppm}$ ketone carbons, lower values when conjugated (s)		