Youngstown State University
Organic Chemistry Spectral Data Sheet

Approximate ^{1}H NMR Chemical Shifts (parts per million)

R_3C-**H**	(alkyl)	0.9 to 1.8	R_3N-C-**H**	(N neighbor)	2.2 to 2.9
C=C-C-**H**	(allylic)	1.6 to 2.6	Cl-C-**H**	(Cl neighbor)	3.1 to 4.1
O=C-C-**H**	(alpha to C=O)	2.1 to 2.5	Br-C-**H**	(Br neighbor)	2.7 to 4.1
NC-C-**H**	(alpha to CN)	2.1 to 3.0	-O-C-**H**	(O neighbor)	3.3 to 3.7
C C **H**	(alkyne)	2.5	R_2N-**H**	(amine)	1 to 3
Ar-C-**H**	(benzylic)	2.3 to 2.8	RO-**H**	(alcohol)	0.5 to 5
C=C-**H**	(alkene)	4.5 to 6.5	Ar-O-**H**	(phenol)	6 to 8
Ar-**H**	(benzene)	6.5 to 8.5	-CO_2**H**	(carboxylic acid)	10 to 13
O=C-**H**	(aldehyde)	9 to 10			

Approximate ^{13}C NMR Chemical Shifts (parts per million)

R**C**H_3	(alkyl)	0 to 35	R**C**H_2Br	(alkyl bromide)	20 to 40
R_2**C**H_2	(alkyl)	15 to 40	R**C**H_2Cl	(alkyl chloride)	25 to 50
R_3**C**H	(alkyl)	25 to 50	R**C**H_2NH_2	(alkyl amine)	35 to 50
R_4**C**	(alkyl)	30 to 40	R**C**H_2OR	(alcohol or ether)	50 to 65
R-**CC**-R	(alkyne)	65 to 90	R**C**N	(nitrile)	110 to 125
R_2**C**=**C**R_2	(alkene)	100 to 150	R**C**O_2R	(acid, ester)	160 to 185
Benzene C	(aromatic)	110 to 175	R**C**HO, R_2**C**O	(ald'hyde, ketone)	190 to 220

Approximate IR Absorption Frequencies (cm^{-1})

Stretching Vibrations

-O-H	(alcohol)	3200 to 3600	C=C	(alkenes)	1620 to 1680
-O-H	(carbox. acid)	2500 to 3600	C=O	(ald., ketones)	1710 to 1750
R_2N-H	(amine)	3350 to 3500	C=O	(acyl halides)	1770 to 1815
sp C-H	(alkynes)	3310 to 3320	C=O	(esters)	1730 to 1750
sp^2 C-H	(alkenes)	3000 to 3100	C=O	(amides)	1680 to 1700
sp^3 C-H	(alkanes)	2850 to 2950			
sp^2 C-O	(carbonyls)	1200	triple bond	(alkynes)	2100 to 2200
sp^3 C-O	(alcoh., ethers)	1025 to 1200	triple bond	(nitriles)	2240 to 2280

Bending Vibrations

RCH=CH_2	(alkenes)	910, 990	Monosubstit'd benzene	730 to 770, 690 to 710
R_2C=CH_2	(alkenes)	890	*ortho*-disubstit'd benzene	735 to 770
R_2C=CHR'	(alkenes)	790 to 840	*meta*-disubstit'd benzene	750 to 810, 680 to 730
			para-disubstituted benzene	790 to 840