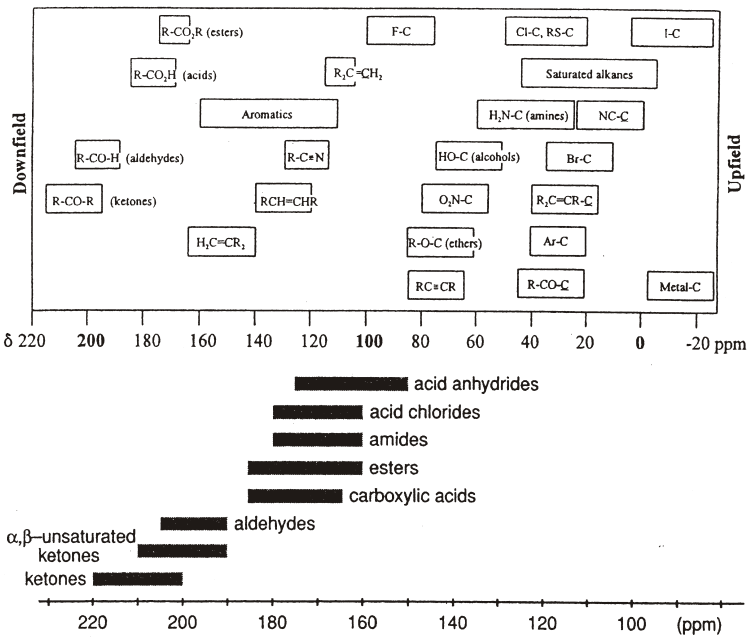
^{13}C nmr Predictions



Chemical shifts of common unsaturated ^{13}C functional groups (δ, ppm from TMS)			
Alkenes		**Aromatics**	
$=CH_2$ (α)	106-117	=CH (benzene)	129
$-\underline{C}H=CH_2$ (β)	138-150	=CH (alkylbenzenes)	127-132
$>\underline{C}=CH_2$ (β)	144-153	=C<	133-138
=CH-	119-144	=CH (naphthalene)	128.1
=C<	124-144	=C< (naphthalene)	137.4
Allenes		**Acetylenes or Alkynes**	
$=CH_2$	74	-C≡C-	~82
=CH-	86	$-C\equiv\underline{C}H$ (α)	70-79
=C=	207-211	$-\underline{C}\equiv CH$ (β)	80-90
Dienes		**Nitrogen groups**	
$=CH_2$	112-118	-C≡N	121
=CH-	~139	>C=NOH	161
=C<	~146	CN^-	178

Values to add to δ128.5 in assigning chemical shifts of substituted benzenes (ppm)									
Substituent	**C-1 (ipso)**	**ortho**	**meta**	**para**	**Substituent**	**C-1 (ipso)**	**ortho**	**meta**	**para**
H	0	0	0	0	OH	26.9	-12.7	1.4	-7.3
CH_3	9.3	0.8	0	-2.9	OCH_3	31.4	-14.4	1.0	-7.7
CH_2CH_3	15.6	-0.4	0	-2.6	$OCOCH_3$	22.4	-7.1	-0.4	-3.2
$CH(CH_2)_2$	20.1	-2.0	0	-2.5	OC_6H_5	29.2	-9.4	1.6	-5.1
$CH(CH_3)_2$	20.2	-2.5	0.1	-2.4	O^-	39.6	-8.2	1.9	-13.6
$C(CH_3)_2$	22.4	-3.1	-0.1	-2.9	CN	-15.4	3.6	0.6	3.9
C_6H_5	13	-1	0.4	-1	NH_2	18.0	-13.3	0.9	-9.8
$CH=CH_2$	9.5	-2.0	0.2	-0.5	$N(CH_3)_2$	23	-16	1	-12
C≡CH	-6.1	3.8	0.4	-0.2	$NHCOCH_3$	11.1	-9.9	0.2	-5.6
CH_2OH	12	-1	0	-1	NO_2	20.0	-4.8	0.9	5.8
COOH	2.1	1.5	0	5.1	F	34.8	-12.9	1.4	-4.5
$COOCH_3$	2.1	1.1	0.1	4.5	Cl	6.2	0.4	1.3	-1.9
COC_6H_5	9.1	1.5	-0.2	3.8	Br	-5.5	3.4	1.7	-1.6
CHO	8.6	1.3	0.6	5.5	I	-32	10	3	1
$COCH_3$	9.1	0.1	0	4.2	$SiMe_3$	13.4	4.4	-1.1	-1.1
COCl	5.8	2.6	1.2	7.4					

Chemical shifts of common saturated ^{13}C functional groups (δ, ppm from TMS)

Alkanes		**Ethers**			
cyclopropanes	0-8	CH_3-O	45-60		
cycloalkanes	2-25	R-CH_2-O	42-70		
R-CH_3	5-25	R_2-CH-O	65-77		
R-CH_2-R	22-45	R_3-C-O	70-83		
R_2-CH-R	30-58	**Carbonyls**			
R_3-C-R	28-50	R-CO-OR	160-177		
Halogens		R-COOH	162-183		
CH_3X	5-25	R-CHO	185-205		
RCH_2X	5-38	R-CO-R	190-220		
R_2CHX	30-62	**Heteroatoms**			
R_3CX	35-75	R-CH_2-S	22-42		
Amines		R-CH_2-P	10-25		
CH_3-N	10-45	Ar-P	120-130		
R-CH_2-N	45-55	Ar-N	130-138		
R_2-CH-N	50-70	Ar-O	130-150		
R_3-C-N	60-75	R-C=N	118-123		

Methyl carbons		Methylene carbons		Methine carbons		Quaternary carbons	
CH_3-C	7-24	-C-CH_2-C	16-30	-C-CH-C	25-30	-C-$\underline{C}$-C	27.7
CH_3-C-NO_2	10-29	-C-CH_2-C-NO_2	12-31	-C-CH-C-NO_2		-C-$\underline{C}$-C-NO_2	
CH_3-C-C=C	13.4	-C-CH_2-C-C=C	22.4	-C-CH-C-C=C		-C-$\underline{C}$-C-C=C	
C=C(CH_3)-CO	15-18	-C-C=C(CH_2)-CO	25-29	-C-C=C(CH)-CO	41.4	-C-C=C($\underline{C}$)-CO	33.0
CH_3-C-O	14-16	-C-CH_2-C-O	27.7	-C-CH-C-O		-C-$\underline{C}$-C-O	
CH_3-C=C	18.7	-C-CH_2-C=C	27-36	-C-CH-C=C	32.3	-C-$\underline{C}$-C=C	33.8
CH_3-C=C-CO	19-24	CH_2-C=C-CO	27-36	CH-C=C-CO	35-47	C-C=C-CO	38-51
CH_3-CO-O-Ar	20.8	-C-CH_2-CO-O-Ar		-C-CH-CO-O-Ar		-C-$\underline{C}$-CO-O-Ar	
CH_3-CO-N-R	21.3	-C-CH_2-CO-N-R	29.0	-C-CH-CO-N-R	34.9	-C-$\underline{C}$-CO-N-R	
CH_3-Ar	25.7	-C-CH_2-Ar	29-30	-C-CH-Ar	26-34	-C-$\underline{C}$-Ar	34-35
CH_3-CO-O-R	20-22	-C-CH_2-CO-O-R	27-29	-C-CH-CO-O-R	34.1	-C-$\underline{C}$-CO-O-R	38.7
CH_3-S	15-20	-C-CH_2-S	32-34	-C-CH-S	33.4	-C-$\underline{C}$-S	45.6
CH_3-CO-Ar	24-28	-C-CH_2-CO-Ar	32-40	-C-CH-CO-Ar	35.2	-C-$\underline{C}$-CO-Ar	43.5
CH_3-N-CO-R	26.1	-C-CH_2-N-CO-R	32-42	-C-CH-N-CO-R	40-48	-C-$\underline{C}$-N-CO-R	49.9
CH_3-CO-R	24-31	-C-CH_2-CO-R	35-45	-C-CH-CO-R	41-52	-C-$\underline{C}$-CO-R	44.3
CH_3-N*	28.3	-C-CH_2-N	37-45	-C-CH-N	43.0	-C-$\underline{C}$-N	
CH_3-N-Ar*	29.9	-C-CH_2-N-Ar	44.2	-C-CH-N-Ar	49.7	-C-$\underline{C}$-N-Ar	
		-C-CH_2-O-H	58-63	-C-CH-O-H	64-67	-C-$\underline{C}$-O-H	68.9
CH_3-O-C=C	51.5	-C-CH_2-O-C=C	61-72	-C-CH-O-C=C	69.2	-C-$\underline{C}$-O-C=C	73.6
CH_3-O-CO-R	51-52	-C-CH_2-O-CO-R	60.4	-C-CH-O-CO-R	67-72	-C-$\underline{C}$-O-CO-R	79.9
CH_3-N$^+$	56.5	-C-CH_2-N$^+$	54-60	-C-CH-N$^+$		-C-$\underline{C}$-N$^+$	
CH_3-O-Ar	54.8	-C-CH_2-O-Ar	63-69	-C-CH-O-Ar	69.3	-C-$\underline{C}$-O-Ar	
CH_3-O-R	50-61	-C-CH_2-O-R	67-72	-C-CH-O-R	72.6	-C-$\underline{C}$-O-R	72.7
		-C-CH_2-NO_2	70-77	-C-CH-NO_2	78-85	-C-$\underline{C}$-NO_2	85.0
		-C-CH_2-CN	10.8	-C-CH-CN	19.8	-C-$\underline{C}$-CN	28.1
		-C-CH_2-I	-1.6	-C-CH-I	20.9	-C-$\underline{C}$-I	43.0
		-C-CH_2-Br	27.6	-C-CH-Br	44.8	-C-$\underline{C}$-Br	62.1
		-C-CH_2-Cl	39.9	-C-CH-Cl	53.7	-C-$\underline{C}$-Cl	66.7

A single figure represents data for only one compound; data given as a range indicate that several model compounds have been found. REMEMBER: These data are only a guide -- actual values will depend upon constraints such as steric and electronic factors, ring strain, etc.

* values increase by ca. 6-8 ppm per degree of substitution; i.e. add 6-8 ppm to this value for a secondary amine, 12-16 for a tertiary, etc.