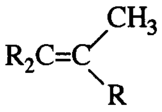
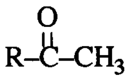
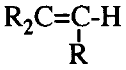
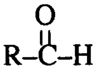
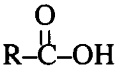
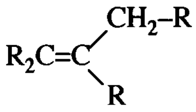
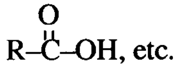
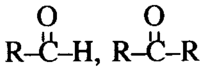
NMR Chemical Shifts

The values for proton and C-13 chemical shifts given below are typical approximate ranges only, and should not be regarded as limiting ranges. A method for approximating proton NMR chemical shifts when more than one shifting influence is present is given on the next page.

Typical Proton NMR Chemical Shifts

Type of Hydrogen		**δ (ppm)**	
Primary (methyl):	$R{-}CH_3$	0.8 – 1.0	Alkane and alkanelike hydrogens
Secondary (methylene):	$R{-}CH_2{-}R$	1.2 – 1.4	
Tertiary (methine):	$R_3C{-}H$	1.4 – 1.7	
Allylic (next to a double bond):	 $R_2C{=}C(CH_3)R$	1.6 – 1.9	Hydrogens adjacent to unsaturated groups
Benzylic (next to a benzene ring):	$Ar{-}CH_2{-}R$	2.2 – 2.5	
Carbonyl (α hydrogens):	 $R{-}\overset{O}{\overset{\|}{C}}{-}CH_3$	2.1 – 2.6	
Chloroalkane:	$R{-}CH_2\text{-}Cl$	3.6 – 3.8	Hydrogens adjacent to electronegative atoms
Bromoalkane:	$R{-}CH_2\text{-}Br$	3.4 – 3.6	
Iodoalkane:	$R{-}CH_2\text{-}I$	3.1 – 3.3	
Alcohol:	$R{-}CH_2\text{-}OH$	3.3 – 4.0	
Ether:	$R{-}CH_2\text{-}OR$	3.3 – 3.9	
Terminal alkene (vinylic):	$R_2C{=}CH_2$	4.6 – 5.0	Hydrogens directly attached to unsaturated groups
Internal alkene (vinylic):	 $R_2C{=}\underset{R}{\underset{\|}{C}}\text{-}H$	5.2 – 5.7	
Alkynic:	$R{-}C{\equiv}C{-}H$	1.7 – 3.1	
Aromatic (benzene ring):	$Ar{-}H$	6.0 – 9.5	
Aldehydic:	 $R{-}\overset{O}{\overset{\|}{C}}{-}H$	9.5 – 9.9	
Carboxylic:	 $R{-}\overset{O}{\overset{\|}{C}}{-}OH$	10.5 – 12	
Alcohol hydroxyl:	$R{-}OH$	0.5 – 5.0	Variable due to hydrogen bonding; depends on concentration and solvent
Amine:	$R{-}NH_2$	0.5 – 5.0	

Typical C-13 NMR Chemical shifts

Type of Carbon		δ (ppm)
Primary:	$R\text{–}CH_3$	5 – 22
Secondary:	$R\text{–}CH_2\text{–}R$	20 – 30
Tertiary:	$R_3C\text{–}H$	30 – 50
Quaternary:	R_4C	35 – 40
Allylic (next to a double bond):	 $R_2C{=}C(CH_2\text{–}R)(R)$	20 – 40
Benzylic (next to a benzene ring):	$Ar\text{–}CH_2\text{–}R$	approx. 30
Chloroalkane:	$R\text{–}CH_2\text{-}Cl$	25 – 50
Bromoalkane:	$R\text{–}CH_2\text{-}Br$	20 – 40
Alcohol:	$R\text{–}CH_2\text{-}OH$	50 - 90
Ether:	$R\text{–}CH_2\text{-}OR$	50 – 90
Alkyne:	$R\text{–}C{\equiv}CH$	65 – 90
Alkene, aromatic:	$C{=}C$	100 – 150
Carboxylic acid and derivatives:	 $R\text{–}\overset{O}{\overset{\|}{C}}\text{–}OH$, etc.	150 – 180
Aldehyde or ketone:	 $R\text{–}\overset{O}{\overset{\|}{C}}\text{–}H$, $R\text{–}\overset{O}{\overset{\|}{C}}\text{–}R$	190 – 210

Approximating Proton NMR Chemical Shifts in More Complex Cases

Consider as an example the molecule $CH_3\text{–}O\text{–}CH_2\text{–}Cl$. The methylene group is shifted by both the O and the Cl, and a corresponding structure isn't in the chemical shift tables. There are two approaches to estimating the chemical shift, one logical and one "quick-and-dirty". Both are approximate at best and tend to give results that are too high; don't expect to hit it on the nose.

The Logical Way: Start by selecting either the O or the Cl, it doesn't matter which, and note how much the atom shifts a methylene group from its "normal" position in an alkane ($R\text{-}CH_2\text{-}R$). Let's use the Cl, and, using shift values from the table, calculate how much the replacement of an R group by Cl changes the chemical shift.

$$\underset{\text{about 3.7 ppm}}{R\text{–}CH_2\text{–}Cl} \xleftarrow{\text{add 2.4 ppm}} \underset{\text{about 1.3 ppm}}{R\text{–}CH_2\text{–}R}$$

Note that the replacement of an R group by Cl causes a downfield shift of about 2.4 ppm. Assume that the same downfield shift will occur in other cases where such a replacement is made. So:

$$\underset{\text{about 6.0 ppm}}{R\text{-}O\text{-}CH_2\text{-}Cl} \xleftarrow{\text{add 2.4 ppm}} \underset{\text{about 3.6 ppm}}{R\text{-}O\text{-}CH_2\text{-}R}$$

The estimated chemical shift is then about 6.0 ppm, whereas the experimental value is found to be 5.2 ppm. It can be seen that the estimated value is high.

The Quick-and-Dirty Way: Simply add the tabulated chemical shifts for the shifting groups. In this case, for $R\text{-}O\text{-}CH_2\text{-}R$ and $R\text{-}CH_2\text{-}Cl$ the table gives 3.6 + 3.7 = 7.3 ppm. The addition will always give a value that is quite a bit too high. Correct it by arbitrarily subtracting 1.5 ppm. This procedure gives an estimate of 7.3 - 1.5 = 5.8 ppm, still too high but close enough.

Sometimes these methods give estimated values that are closer to the experimental values, but there is no reliable way to predict when this might be the case.