Predicting the chemical shift of proton/s on a sp^3 carbon in a ^1H NMR spectrum

Step one: Find the all chemically non-equivalent proton/s.

When predicting chemical shifts, you consider the chemically non-equivalent proton/s one at a time.

Step two: Find the starting point for each chemically non-equivalent proton/s.

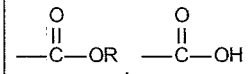
The starting point is dependent upon if the proton/s are attached to a methyl, a methene or a methine.

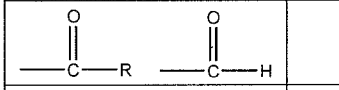
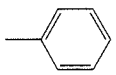
If the protons are attached to a methyl (XCH_3) the starting point is 0.9 ppm.
If the protons are attached to a methene (XCH_2X) the starting point is 1.3 ppm.
If the proton is attached to a methine (X_3CH) the starting point is 1.5 ppm.

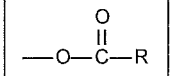
X can represent anything but a H or D .

Step three: What is X?

Identify all groups (X) that are directly bonded to the carbon atom that bears the proton/s of interest. Be carful with esters because they have two sides, the carbonyl side and the acyoxy side.

Group (X)	Increment (ppm)
—CH_3 (or any alkyl group)	0.0
—$CH{=}CH_2$ (or any alkene group)	0.9
—$C{\equiv}CR$; —$C{\equiv}CH$	0.9
—SR, —SH	1.2
	1.2

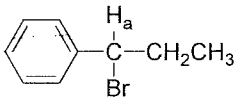
Group (X)	Increment (ppm)
—$C{\equiv}N$	1.2
	1.2
—NH_2, —NHR, —NR_2	1.2
—I	1.3
—Ph 	1.4

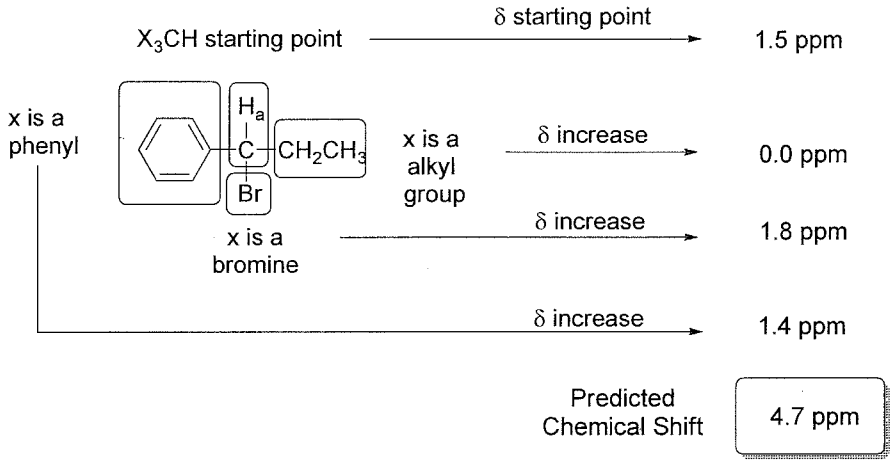
Group (X)	Increment (ppm)
—Br	1.8
—Cl	2.1
—OR, —OH	2.4
	2.8
—OPh	3.0
—F	3.2

Step four: Add the values together.

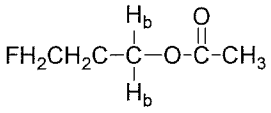
When predicting chemical shifts, you need to watch for *remote* (not geminal) electronegative group/s. If a substituent has a remote electronegative group, an asterisk (*) is add to the chemical shift increment indicating that the chemical shift increment will be increased. Adding the starting point and all the X values together (including the asterisk) will provide the approximate chemical shift of the proton of interest.

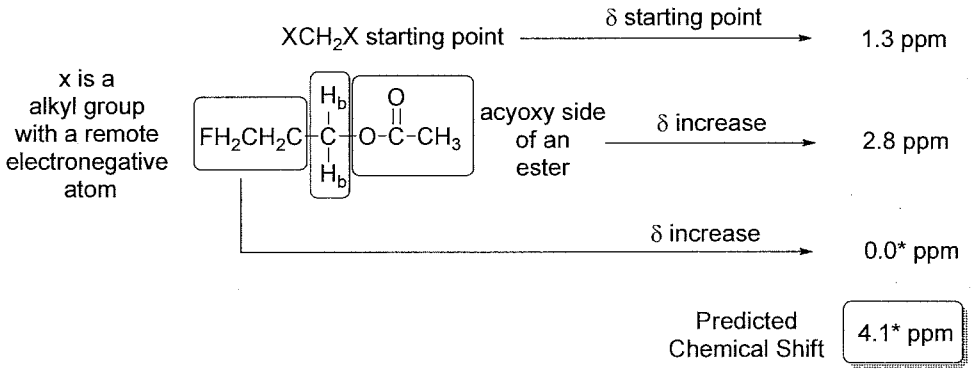
What is the predicted chemical shift (δ) of proton Ha?





What is the predicted chemical shift (δ) of proton Hb?





Thank-you Dr. J. R Walker at Oregon State University for the foundation of this document