Answer on Question #41244 – Chemistry – Organic Chemistry

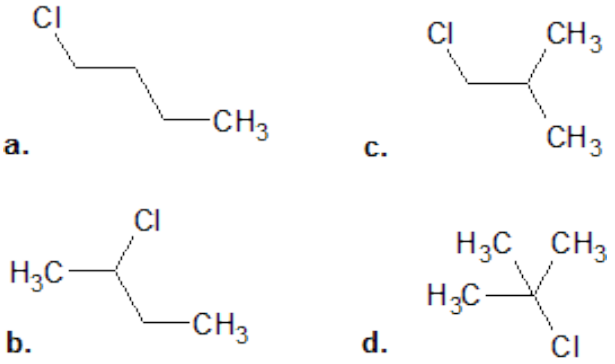
Question:

Draw the structure of the C_4H_9Cl isomer given the following proton NMR data:
doublet d 1.04 (6H)
multiplet d 1.95 (1H)
doublet d 3.35 (2H)

Explain your reasoning.

Answer:

C_4H_9Cl corresponds to the general formulae **$C_nH_{2n+1}Cl$**, which represents alkyl chlorides. The following isomers of can be drawn for **C_4H_9Cl** (a, b, c, d respectively):



Fig(1). Possible isomers of C4H9Cl

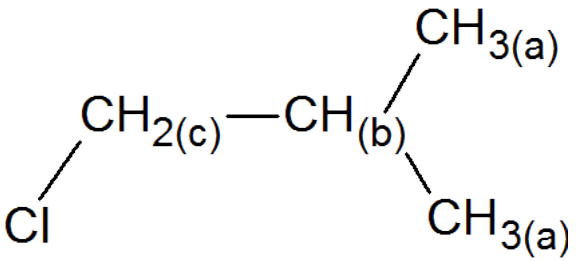
The NMR data must be analyzed. The multiplicity of the signal relates to the number of adjacent hydrogen atoms as **N = n – 1**, where **N** is number of adjacent hydrogen atoms, **n** is the multiplicity of the signal. The value after multiplicity refers to the frequency of the signal and is measured in parts per million. The greatest frequency corresponds to an atom which has an adjacent acceptor atom (atom with great electronegativity). It is said that signal is in the weak field in that case. The number of hydrogen atoms that generate the signal is noted in brackets.

The following table will help to determine the structure of unknown isomer:

Serial number of signal	Multiplicity **n**	Amount of adjacent hydrogen atoms **N = n -1**	Frequency, field	Amount of hydrogen atoms that generate the signal, H
1	doublet **n = 2**	**N = 1**	1.04, **strong field**	**6 H**
2	multiplet **n > 5**	**N > 4**	1.95, **strong field**	**1 H**
3	doublet **n = 2**	**N = 1**	3.35, **weak field**	**2 H**

Corresponding isomer must have six analogous hydrogen atoms, surrounded by one hydrogen atom. The third signal originates from two hydrogen atoms bonded with carbon that is connected with chlorine atom. Chlorine has great electronegativity value, so the signal of adjacent protons is shifted in the weak filed (3.35 ppm). No doubt that only one isomer **d.**, namely **1-chloro-2-methylpropane** is suitable.

Signals **1, 2, 3** can be correlated with hydrogen atoms **(a), (b), (c)** respectively (Fig2).



Fig(2). Different hydrogen atoms in 1-chloro-2-methylpropane