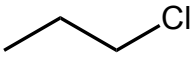
^{1}H NMR Spectroscopy

1. Consider the structure of **1-chloropropane**.



Answer the following questions related to draw a representative ^{1}H NMR spectrum of 1-chloropropane.

A. How many signals should be present? **Three signals**

B. List the approximate chemical shifts of each signal from downfield to upfield.

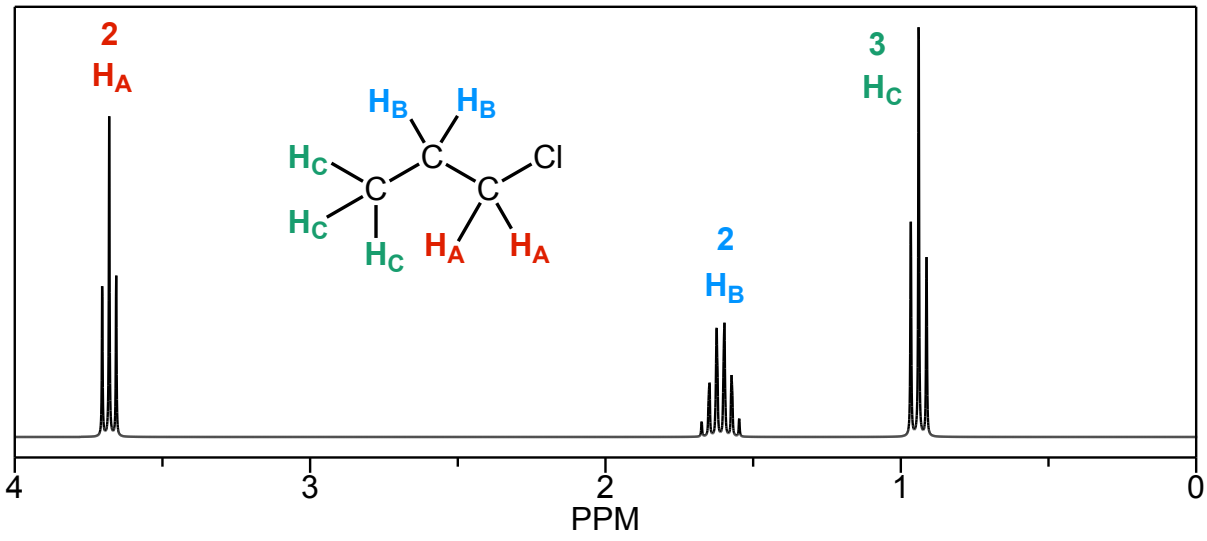
H_A (3-4 ppm) ; H_B (1-2 ppm) ; H_C (~1 ppm)

C. What would the integration of the peaks be?

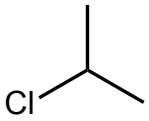
2 : **2** : **3**

D. What is the expected splitting pattern of each signal?

H_A (triplet) ; H_B (sextet) ; H_C (triplet)



2. Consider the structure of **2-chloropropane**.



Answer the following questions related to draw a representative ^{1}H NMR spectrum of 2-chloropropane.

A. How many signals should be present? **2 signals**

B. List the approximate chemical shifts of each signal from downfield to upfield.

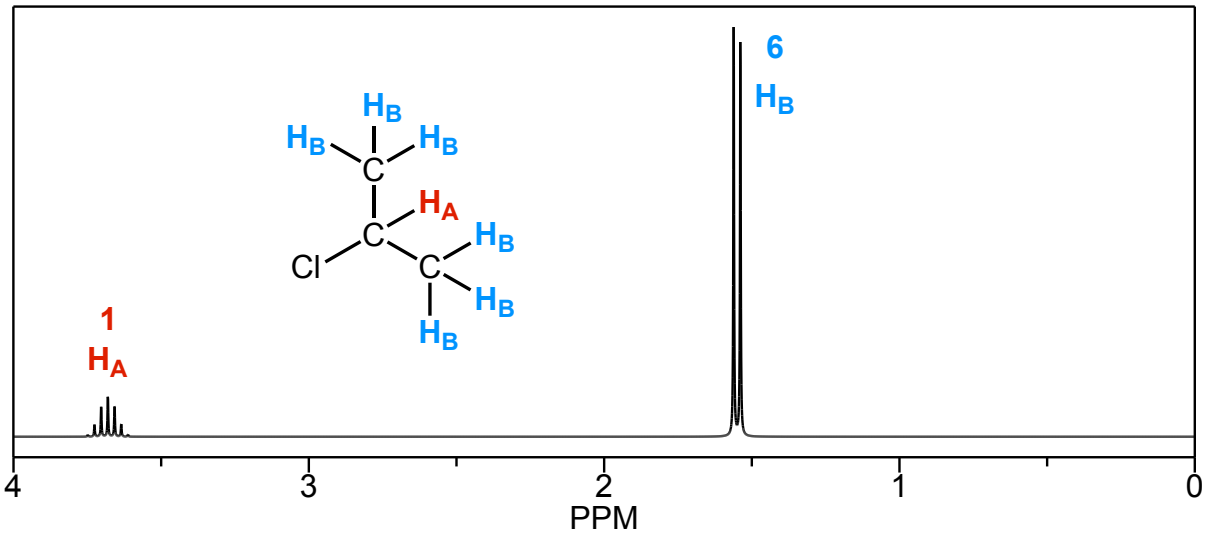
H_A (3-4 ppm) ; **H_B** (1-2 ppm)

C. What would the integration of the peaks be?

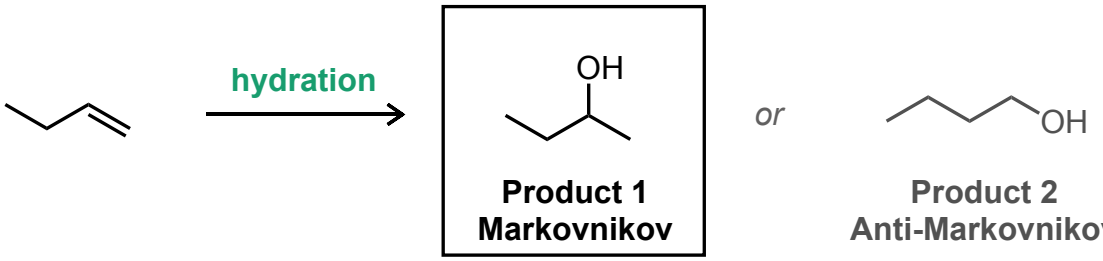
1 : **6**

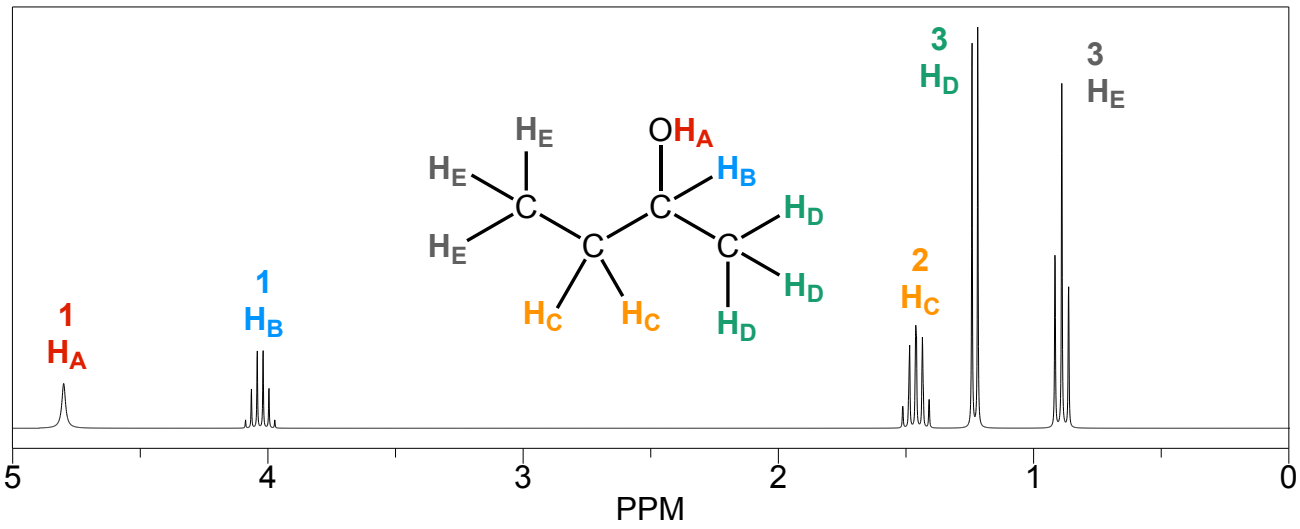
D. What is the expected splitting pattern of each signal?

H_A (septet because of 6 adajcent H_B, 6 + 1 = 7) ; **H_B** (doublet)



3. A hydration (addition of H and OH) reaction has taken place on an alkene starting material. **Use the ^{1}H NMR spectrum** of the unknown product **to determine** whether the **Markokvnikov** or **anti-Markovnikov** product has formed.





A. Does the number of signals indicate one product over the other? Explain.

No.
Product 1: Expect 5 signals
Product 2: Expect 5 signals

B. Do the chemical shifts observed in the NMR indicate one product over the other? Explain.

No. We would expect both products to have similar shifts since they are both alcohols

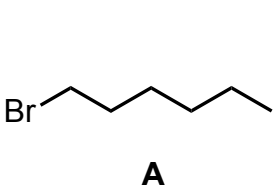
C. Does the integration of signals indicate one product over the other? Explain.

Yes.
Product 1: Expect 1 : 1 : 2 : 3 : 3 <----- **agrees with spectrum**
Product 2: Expect 1 : 2 : 2 : 2 : 3

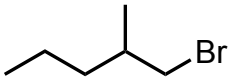
D. Does the observed splitting indicate one product over the other? Explain?

Yes, the splitting observed indicates we have formed **product 1**, but we often utilize splitting as our last parameter.

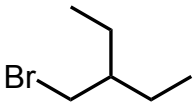
4. Which constitutional isomer is represented by ^{1}H NMR spectrum below?



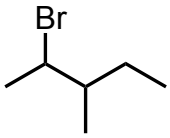
A



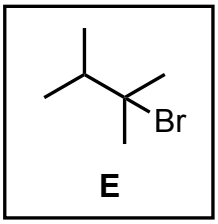
B



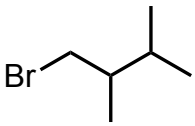
C



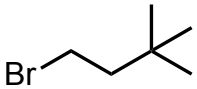
D



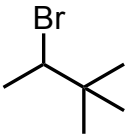
E



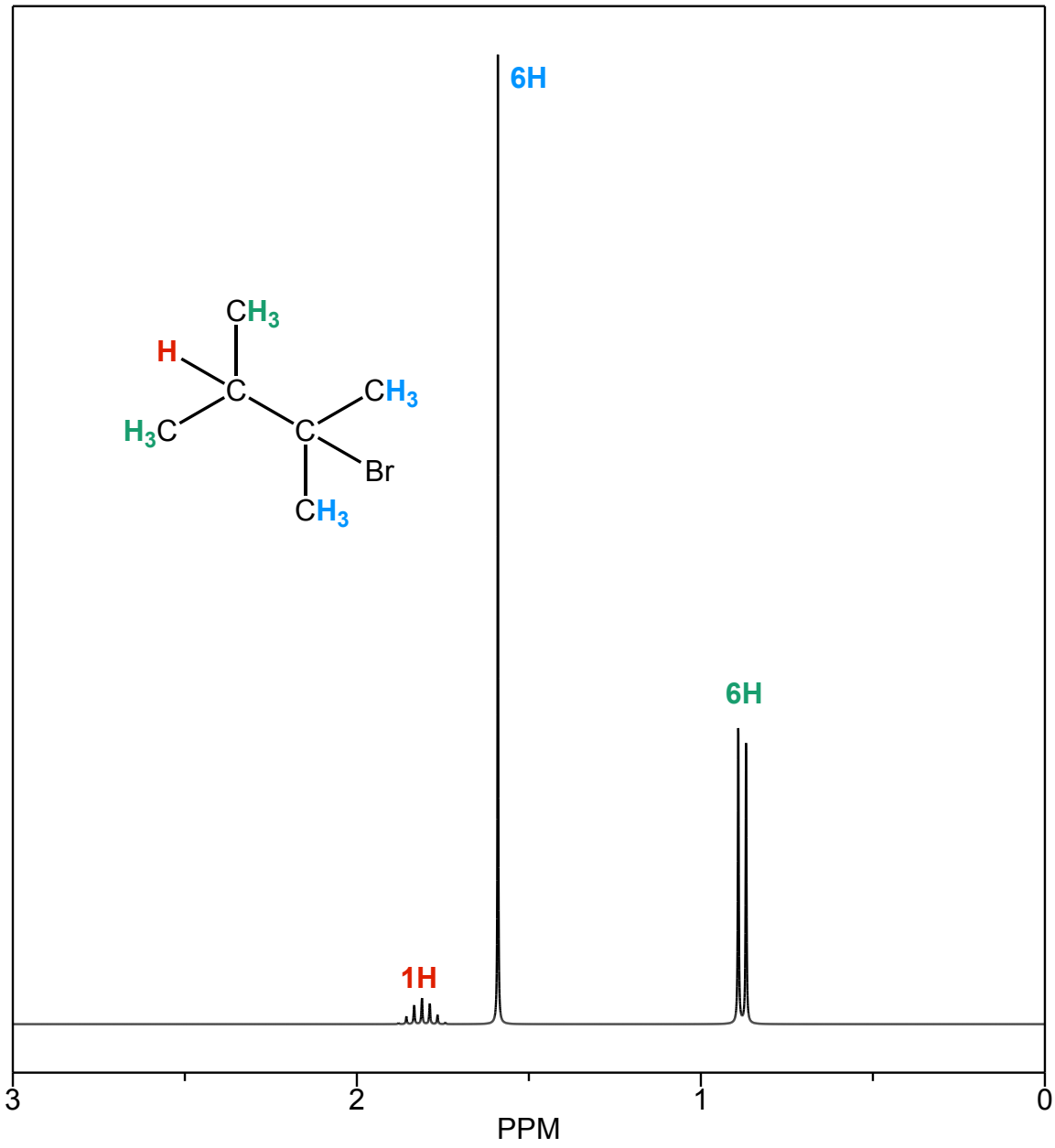
F



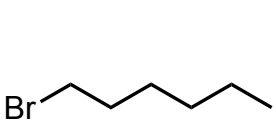
G



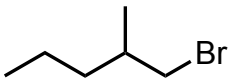
H



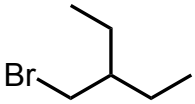
5 Which constitutional isomer is represented by ^{1}H NMR spectrum below?



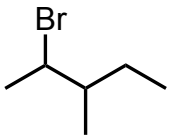
A



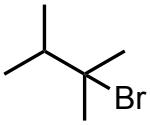
B



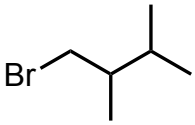
C



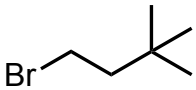
D



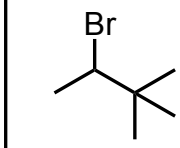
E



F



G



H