جامعة تكريت
كلية التربية للبنات
قسم الكيمياء

التشخيص العضوي

المحاضرة (3)

الازاحات الكيميائية وامثلة تطبيقية

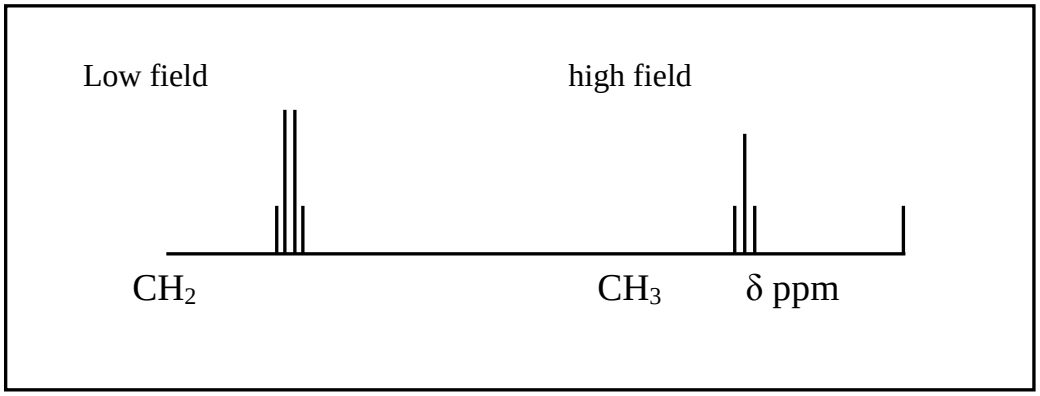
أعـداد

أ.د. سلوى عبد الستار جبار

s.abd@tu.edu.iq

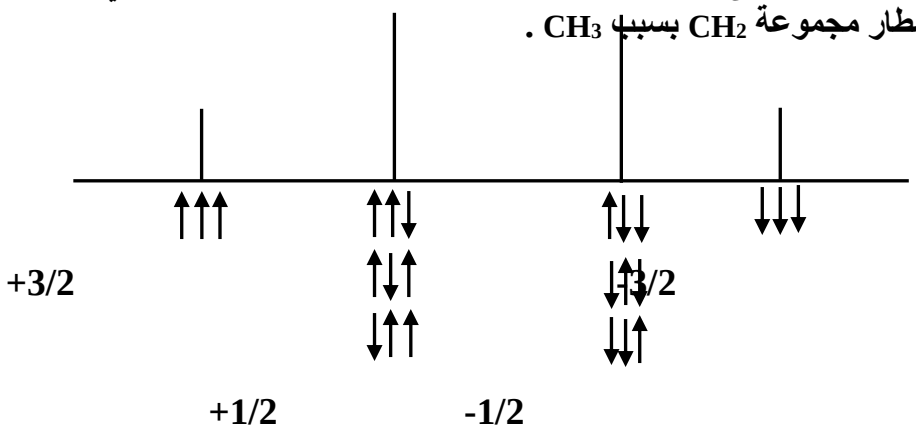
الطيف لأنها متصلة بمجموعه ساحبة وهو البروم الذي يعمل على تعرية بروتونات مجموعة المثيلين

ويقلل حجبها وبالتالي تظهر أشارتها بالمجال الواطئ من طيف ^{1}HNMR أي بإزاحة كيميائية δ كبيرة .

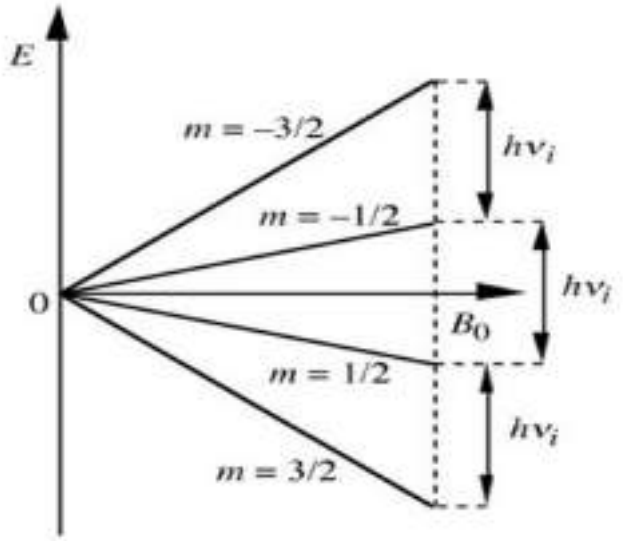


توجد أربع حالات لدوران بروتونات CH_3 أو أربع طاقات(3/2- , 1/2- , 1/2+ , 3/2+) مختلفة تؤدي إلى شطر قمة CH_2 إلى أربعة خطوط أو انشطارات بنسبة 1:3:3:1 وكالاتي :

*** انشطار مجموعة CH_2 بسبب CH_3 .**

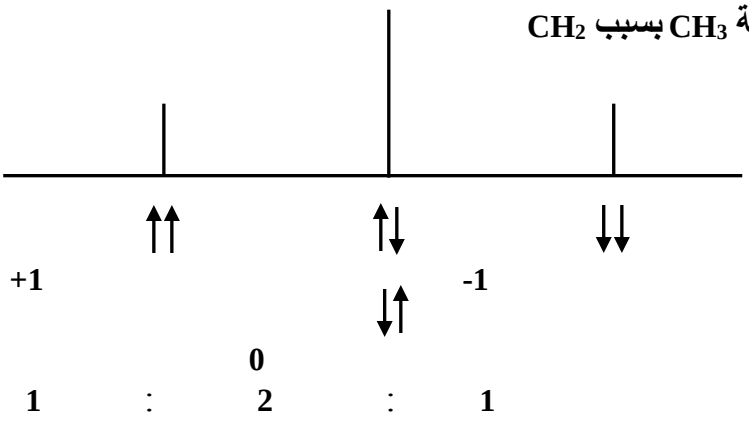


رسم يوضح مستويات الطاقة لبرم بروتون ما قيمة I=3/2 وحسب القانون (2I+1) تكون هناك أربع حالات للطاقة وكالاتي :



1 : 3 : 3 : 1

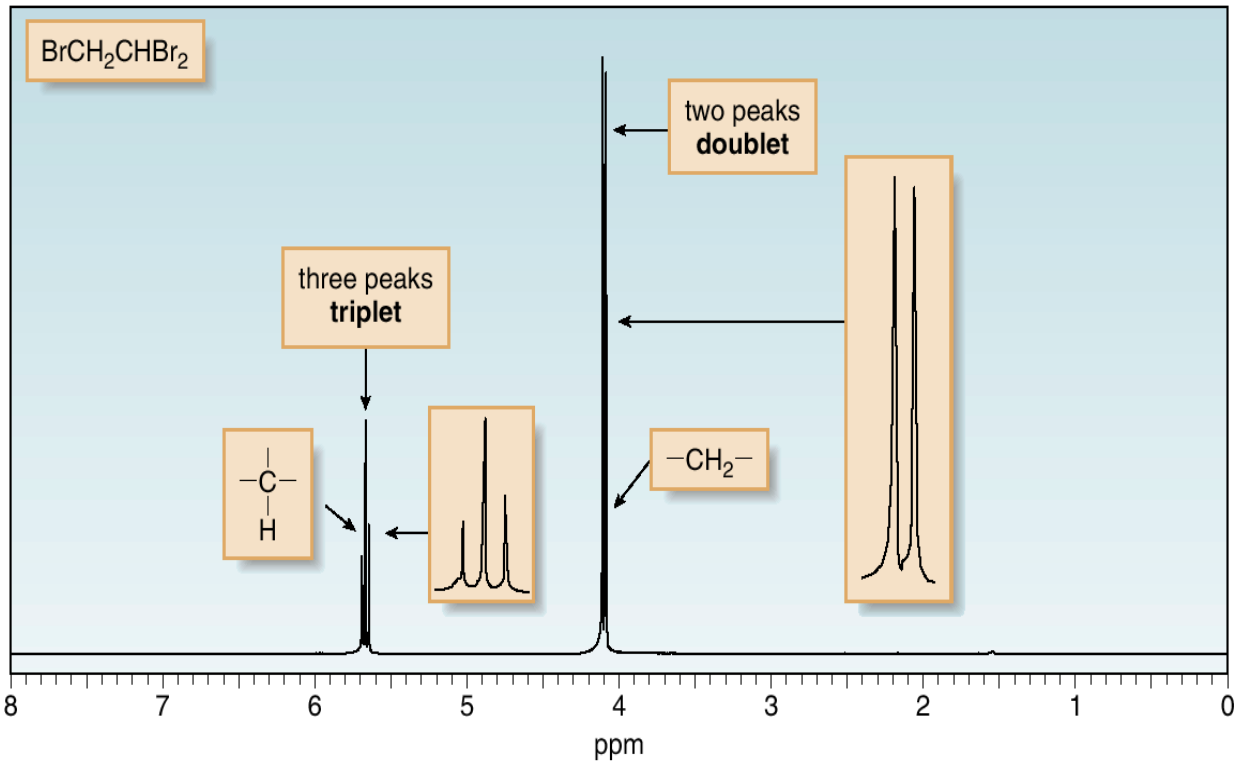
*** انشطار مجموعة CH_3 بسبب CH_2**



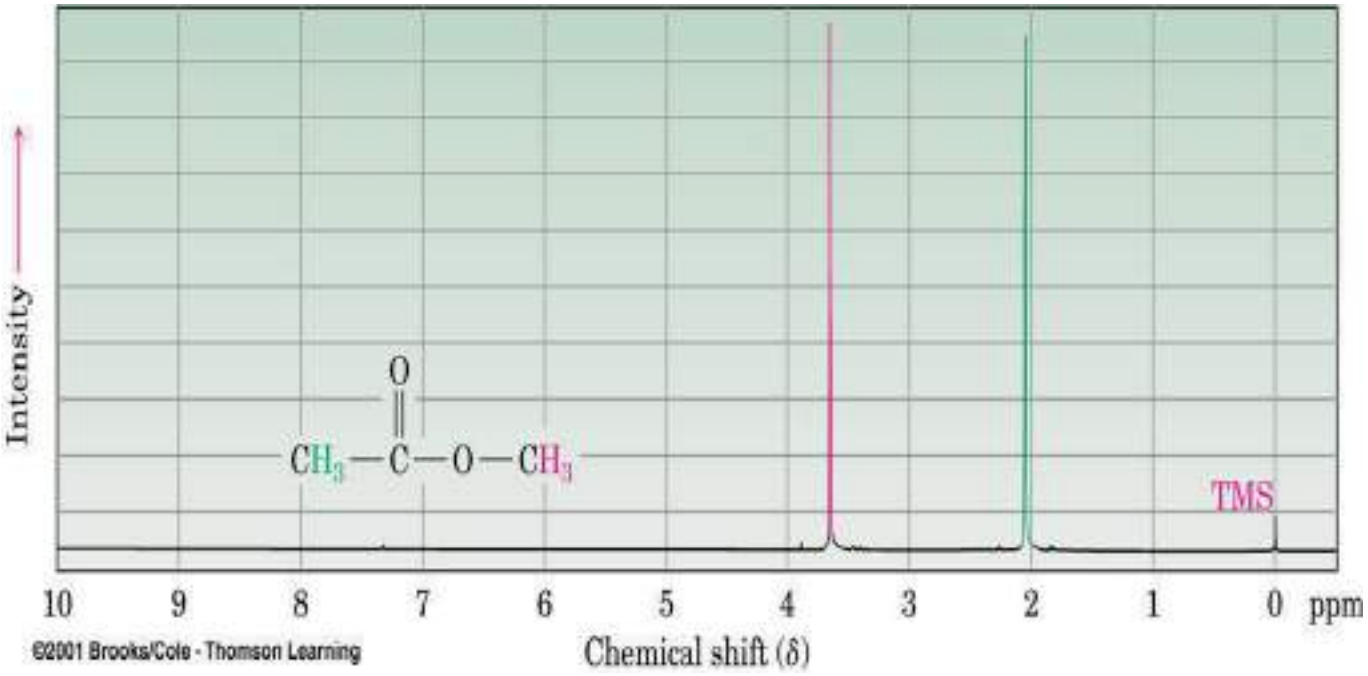
1 : 2 : 1

البروتونات على ذرات مغايرة protons on the hetero atoms

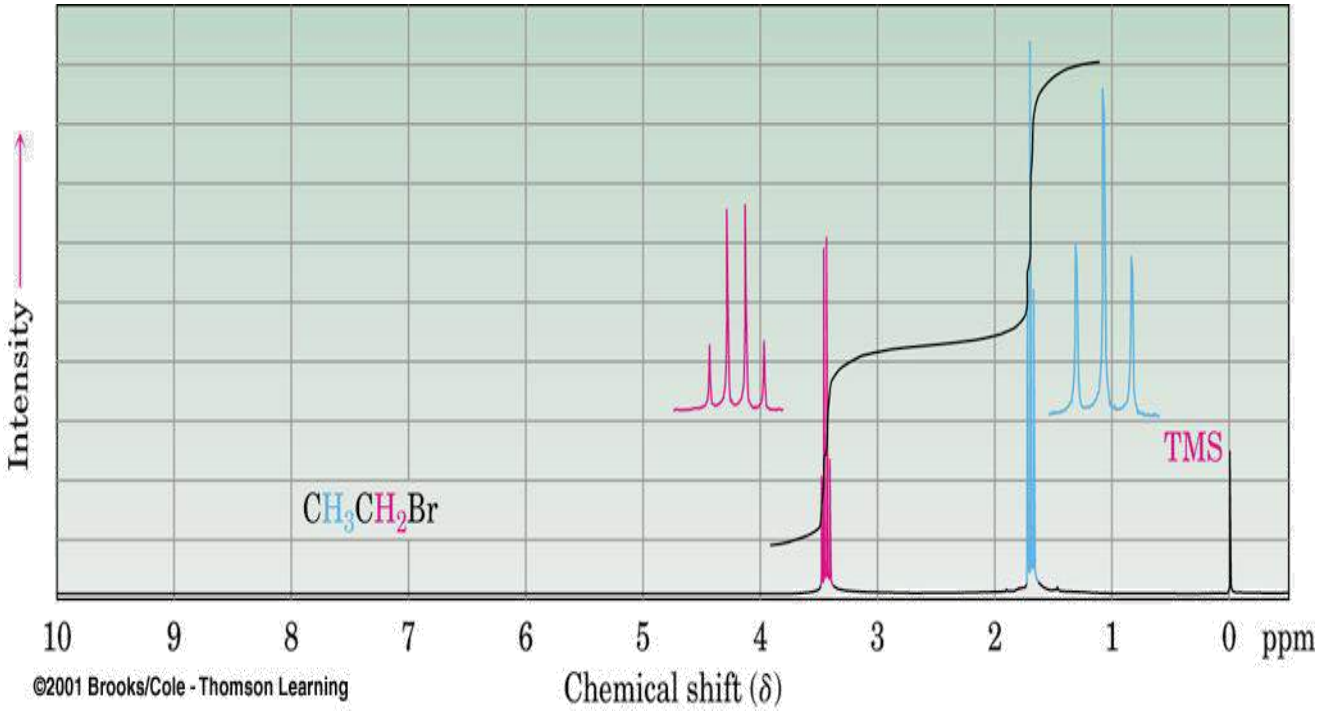
Examples on signals for some compounds in NMR spectroscopy



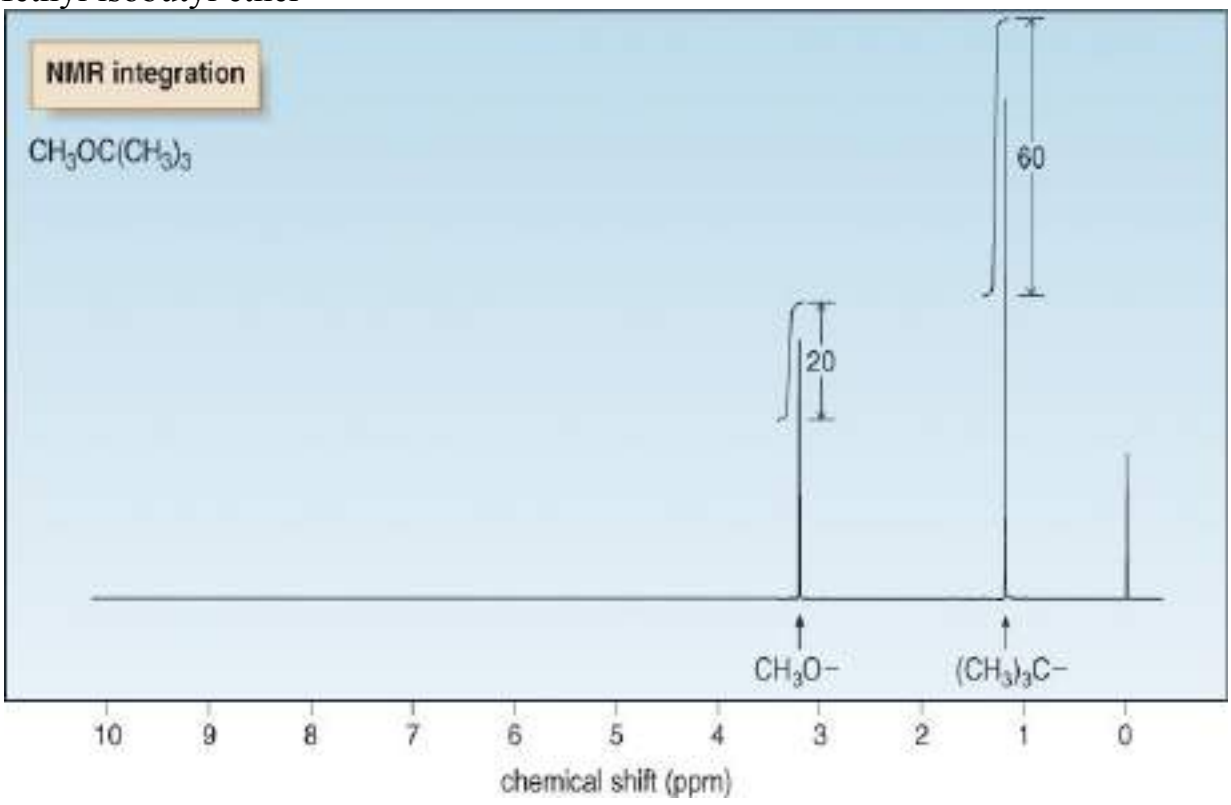
Methyl acetic acid



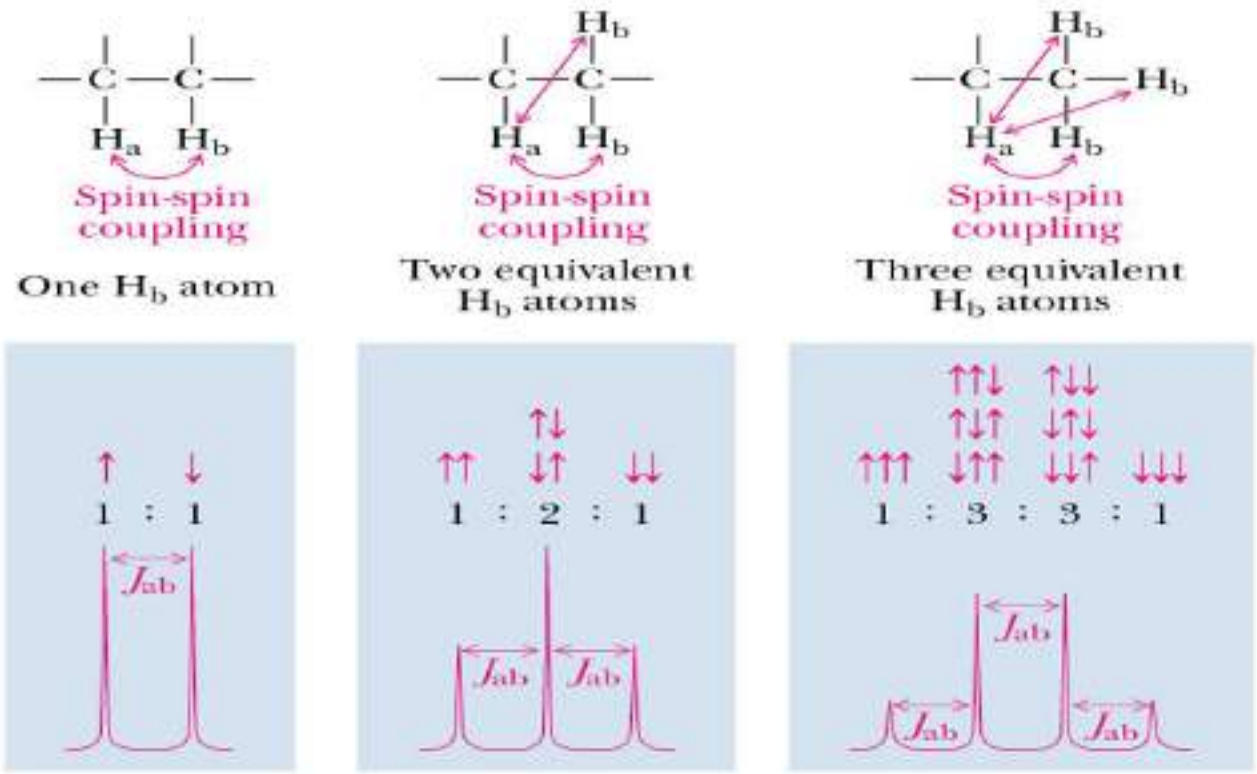
Bromo ethane



Methyl isobutyl ether

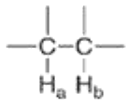
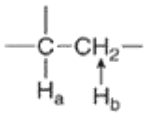
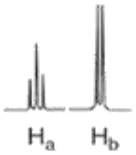
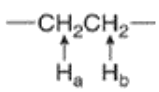
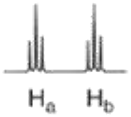
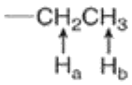
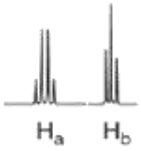
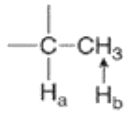
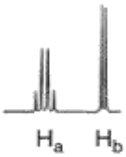


1H NMR—Spin-Spin Splitting



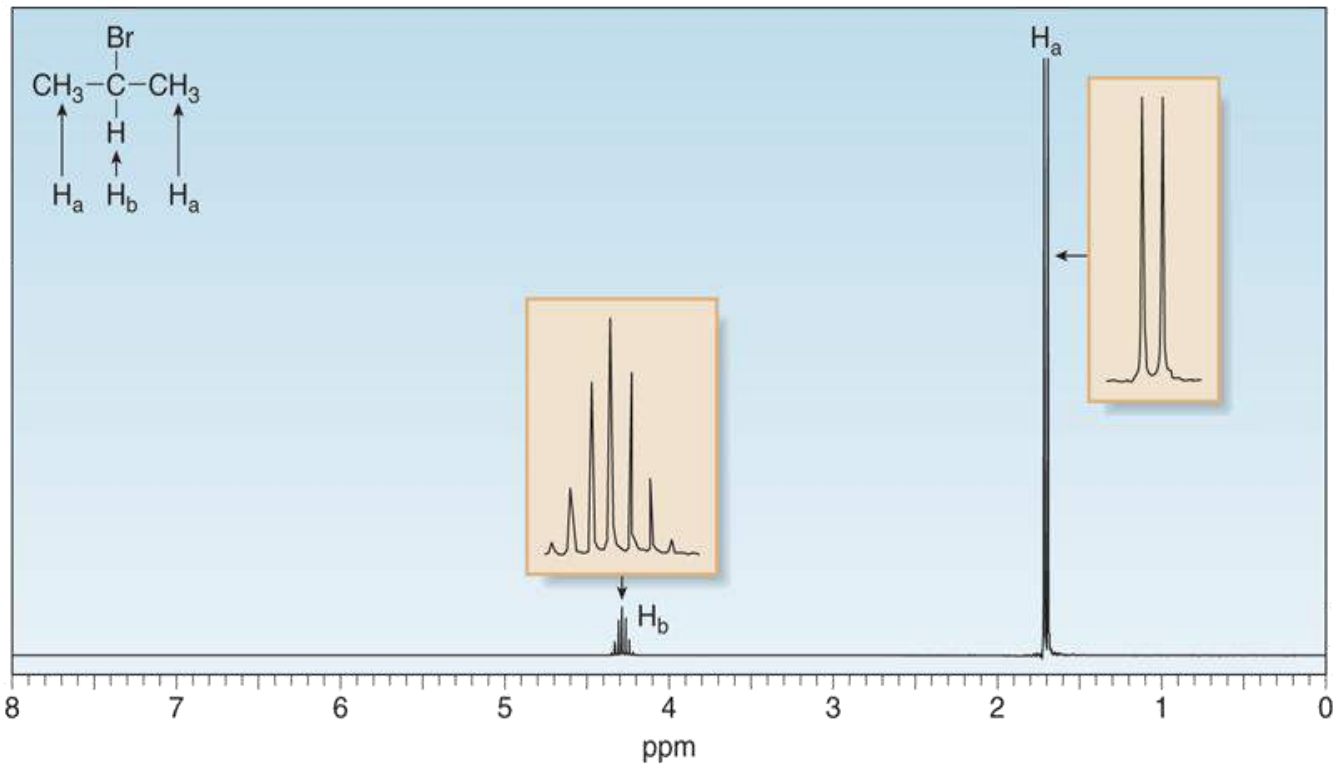
Observed splitting in signal of H_a

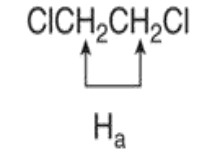
Table 14.4 Common Splitting Patterns Observed in ^{1}H NMR

Example	Pattern	Analysis (H_a and H_b are not equivalent.)
[1] 		• H_a: one adjacent H_b proton ----→ two peaks ----→ a **doublet** • H_b: one adjacent H_a proton ----→ two peaks ----→ a **doublet**
[2] 		• H_a: two adjacent H_b protons ----→ three peaks ----→ a **triplet** • H_b: one adjacent H_a proton ----→ two peaks ----→ a **doublet**
[3] 		• H_a: two adjacent H_b protons ----→ three peaks ----→ a **triplet** • H_b: two adjacent H_a protons ----→ three peaks ----→ a **triplet**
[4] 		• H_a: three adjacent H_b protons ----→ four peaks ----→ a **quartet*** • H_b: two adjacent H_a protons ----→ three peaks ----→ a **triplet**
[5] 		• H_a: three adjacent H_b protons ----→ four peaks ----→ a **quartet*** • H_b: one adjacent H_a proton ----→ two peaks ----→ a **doublet**

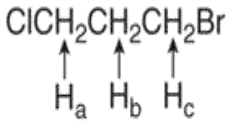
*The relative area under the peaks of a quartet is 1:3:3:1.

2-Bromo propane

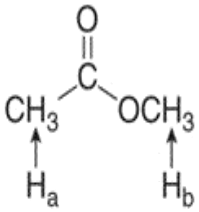




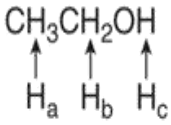
1 type of H
1 NMR signal



3 types of H's
3 NMR signals



2 types of H's
2 NMR signals



3 types of H's
3 NMR signals

Position of signals (chemical shift): what types of hydrogens.

Primary	0.9ppm
Secondary	1.3ppm
Tertiary	1.5 ppm
Aromatic	6-8.5 ppm
Benzyl	2.2-3ppm
Chlorides	3-4 ppm
Bromides	2.5-4ppm
Iodides	2-4ppm
Alcohols	3.4-4ppm
Alcohols	1-5.5ppm
Aldehydes	9-10ppm
Phenols	10-12ppm
Carboxylic acids	11-13ppm

Each peak represents a fragment of the molecule

Peak carries three critical pieces of information

Integration: how many hydrogens on that fragment

Chemical shift: functional group on or next to the fragment

Multiplicity: how many next-door hydrogens

n + 1 rule

The number of peaks in a multiplet can give additional information about the structure.

The splitting of peaks is caused by the neighbouring carbon's hydrogen atoms.

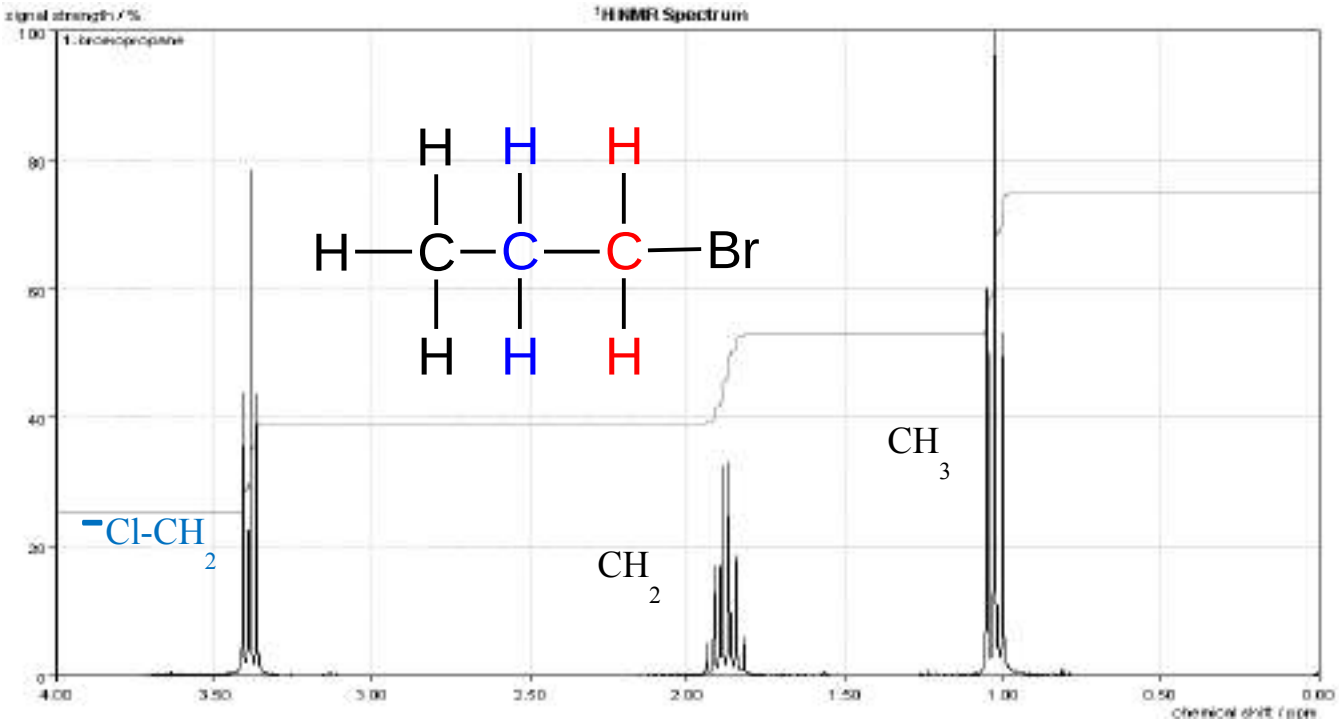
Protons in the same environment are said to be equivalent and as such behave as one proton.

This follows the n + 1 rule.

n is the number of hydrogen atoms attached to the next-door carbon

- n + 1 is how many peaks will be seen in the cluster

Bromopropane



Hydrogen and Carbon Chemical Shifts