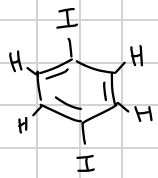
27.10.2025

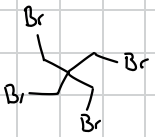
2/2 Great work!

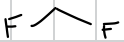
Jigsaw 2A

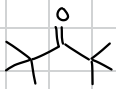
Exo 1

a. 

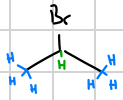
b. 

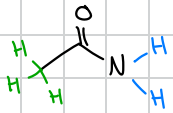
c. 

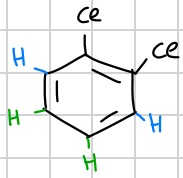
d. 

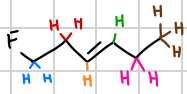
e. 

Exo 2

a.  ⇝ 2 signals

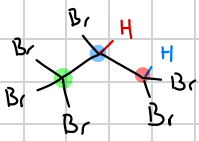
b.  ⇝ 2 signals

c.  ⇝ 2 signals

d.  ⇝ 6 signals

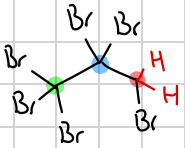
Exo 3

a.



$\rightsquigarrow$ ^1H : 2 signals

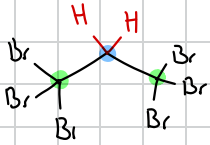
$\rightsquigarrow$ ^{13}C : 3 signals



$\rightsquigarrow$ ^1H : 1 signal

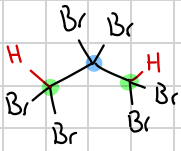
$\rightsquigarrow$ ^{13}C 3 signals

b.



$\rightsquigarrow$ ^1H : 1 signal

$\rightsquigarrow$ ^{13}C : 2 signals



$\rightsquigarrow$ ^1H : 1 signal

$\rightsquigarrow$ ^{13}C : 2 signals

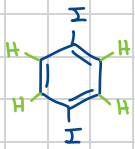
Structural analysis: Jigsaw 2A

2/2 Nice work!

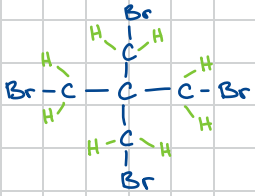
1. The following compounds all exhibit a single line in their ^1H NMR spectra. Deduce their structures.

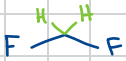
   a. $C_6H_4I_2$ b. C_3H_9N c. $C_5H_8Br_4$

   d. CH_2F_2 e. $C_9H_{14}O$

a) 

b) 

c) 

d) 

e) The insaturation degree is:

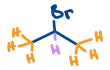
$ID = \frac{1}{2}(2 \cdot 9 - 14 + 2) = 3 \Rightarrow$ the molecule must have 3 insaturations

However, we cannot find a configuration that has all hydrogens equivalent

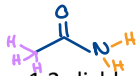
It was supposed to be H18....ooops....

2. How many different signals will you see in a ^1H spectrum in the following molecules?

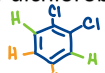
   a. $CH_3CBrHCH_3$ ⇒ 2 signals



   b. $CH_3C(O)NH_2$ ⇒ 2 signals

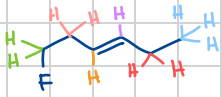


   c. 1,2-dichlorobenzene



⇒ 2 signals

   d. $CH_2FCH_2CHCHCH_2CH_3$ ⇒ 6 signals

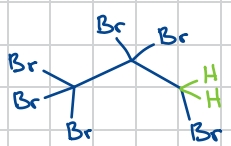


3. ^1H and ^{13}C NMR spectra were recorded for two isomers of $C_3H_2Br_6$. The ^{13}C spectra contain peaks at three distinct chemical shifts. Isomer 1 has one distinct ^1H chemical shift and isomer 2 has two.

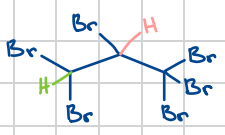
   a. Deduce the structures of the two compounds.

   b. Predict the number of chemical shifts in the ^1H and ^{13}C spectra of the other two isomers of $C_3H_2Br_6$.

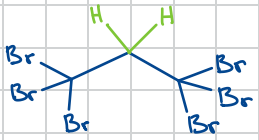
a) ① ^1H: one peak
^{13}C: three peaks ⇒



② ^1H: 2 peaks
^{13}C: 3 peaks ⇒

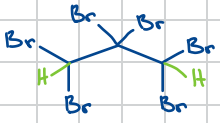


b) #1



^1H: 1 chem shift
^{13}C: 2 chem shifts

#2



^1H: 1 chem shift
^{13}C: 2 chem shifts

2/2 Good job!

CH-314 Structural Analysis
ruben.rodriguezmadrid@epfl.ch
ray.cowen@epfl.ch

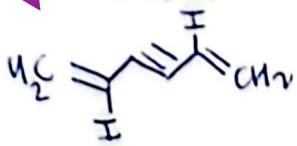
This seems to work too, but don't forget about aromatics! We were thinking of 1,4-diiodobenzene

Jigsaw 2A

Hore Section 2.2. Nuclear shielding

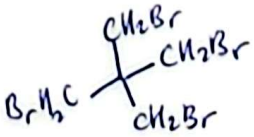
1. The following compounds all exhibit a single line in their ^{1}H NMR spectra. Deduce their structures.

a. $C_6H_4I_2$

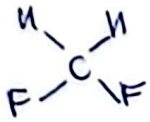


b. C_3H_9N

c. $C_5H_8Br_4$



d. CH_2F_2



e. $C_9H_{14}O$

Good catch on the labile 1H! The protons attached to the N are exchangeable so they won't give a sharp peak like we're used to seeing for 1H. Labile 1H peaks can be missing/obscured in the solvent signal or can be very broad.

2. How many different signals will you see in a ^{1}H spectrum in the following molecules?

a. $CH_3CBrHCH_3$ 2 (7 peaks + 2 peaks)

b. $CH_3C(O)NH_2$ 1 (1 peak)

c. 1,2-dichlorobenzene 2 (4peaks + 4peaks)

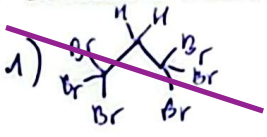
d. $CH_2FCH_2CHCHCH_2CH_3$ 5 (3peaks + 5 + 4 + 4 + 3)

3. ^{1}H and ^{13}C NMR spectra were recorded for two isomers of $C_3H_2Br_6$. The ^{13}C spectra contain peaks at three distinct chemical shifts. Isomer 1 has one distinct ^{1}H chemical shift and isomer 2 has two.

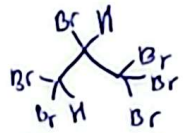
Due to symmetry, this would only have two distinct 13C shifts. Isomer 1 should have both protons on one of the terminal C

a. Deduce the structures of the two compounds.

1)



2)



b. Predict the number of chemical shifts in the ^{1}H and ^{13}C spectra of the other two isomers of $C_3H_2Br_6$.

	^{1}H	^{13}C
isomer 1)	1	2
~~isomer 2)~~ 2 signals with 2 chemical shifts		3

Both other isomers should have one 1H shift and two 13C shifts due to symmetry; one has both protons on the central C and the other has one proton on each terminal C