13.0 Unit Preview

13.1 Nuclear Magnetic Resonance Spectroscopy

13.1 Exercises

Questions

Q13.1.1

If in a field strength of 4.7 T, H\textsuperscript{1} requires 200 MHz of energy to maintain resonance. If atom X requires 150 MHz, calculate the amount of energy required to spin flip atom X’s nucleus. Is this amount greater than the energy required for hydrogen?

Q13.1.2

Calculate the energy required to spin flip at 400 MHz. Does changing the frequency to 500 MHz decrease or increase the energy required? What about 300 MHz.

Solutions

S13.1.1

\[ E = h\nu \]

\[ E = (6.62 \times 10^{-34})(150 \text{ MHz}) \]

\[ E = 9.93 \times 10^{-26} \text{ J} \]

The energy is equal to 9.93x10\textsuperscript{-26} J. This value is smaller than the energy required for hydrogen (1.324 \times 10^{-25} \text{ J}).

S13.1.2

\[ E = h\nu \]

\[ E = (6.62 \times 10^{-34})(400 \text{ MHz}) \]

\[ E = 2.648 \times 10^{-25} \text{ J} \]
The energy would increase if the frequency would increase to 500 MHz, and decrease if the frequency would decrease to 300 MHz.

13.2 The Nature of NMR Absorptions

13.2 Exercises

Questions

Q13.2.1

2-chlorobutene shows 4 different hydrogen signals. Explain why this is.

Solutions

S13.2.1

The same colors represent the same signal. 4 different colors for 4 different signals. The hydrogen on the alkene would give two different signals.

13.3 Chemical Shifts

13.3 Exercises

Questions

Q13.3.1

The following peaks were from a $^1H$ NMR spectra from a 400 MHz spectrometer. Convert to $\delta$ units

A. CHCl$_3$ 1451 Hz

B. CH$_3$Cl 610 Hz
C. CH₃OH 693 Hz
D. CH₂Cl₂ 1060 Hz

Q13.3.2

Butan-2-one shows a chemical shift around 2.1 on a 300 MHz spectrometer in the H¹ NMR spectrum.

A. How far downfield is this peak from TMS in Hz?
B. If the spectrum was done with a 400 MHz instrument, would a different chemical shift be seen?
C. On this new 400 MHz spectrum, what would be the difference in Hz from the chemical shift and TMS?

Solutions

S13.3.1

A. 3.627 ppm
B. 1.525 ppm
C. 1.732 ppm
D. 2.65 ppm

S13.3.2

A. Since TMS is at 0 δ = 0 Hz for reference, the difference between the two would be 630 Hz
B. No not a different chemical shift, but a different frequency would be seen, 840 Hz
C. 840 Hz

13.4 ¹³C¹³C NMR Spectroscopy: Signal Averaging and FT-NMR

13.5 Characteristics of ¹³C¹³C NMR Spectroscopy

13.7 Uses of ¹³C¹³C NMR Spectroscopy

13.8 ¹H¹H NMR Spectroscopy and Proton Equivalence
13.8 Exercises

Questions

Q13.8.1

How many non-equivalent hydrogen are in the following molecules; how many different signals will you see in a $^1H$ NMR spectrum.

A. CH$_3$CH$_2$CH$_2$Br
B. CH$_3$OCH$_2$C(CH$_3$)$_3$
C. Ethyl Benzene
D. 2-methyl-1-hexene

Solutions

S13.8.1

A. 3; B. 3; C. 5; D. 7

13.9 Chemical Shifts in $^1H$ NMR Spectroscopy

13.9 Exercises

Questions

Q13.9.1

The following have one $^1H$ NMR peak. In each case predict approximately where this peak would be in a spectra.
Q13.9.2

Identify the different equivalent protons in the following molecule and predict their expected chemical shift.

![Molecule Image]

Solutions

S13.9.1

A. 5.20 δ; B. 1.50 δ; C. 6.40 δ; D. 1.00 δ

S13.9.2

There are 6 different protons in this molecule

The shifts are (close) to the following: (a) 2 δ; (b) 6 δ; (c) 6.5 δ; (d) 7 δ; (e) 7.5 δ; (f) 7 δ
13.10 Integration of 1H NMR Absorptions: Proton Counting

13.10 Exercises

Questions

Q13.10.1

Predict how many signals the following molecule would have? Sketch the spectra and estimate the integration of the peaks.

Solutions

S13.10.1

There will be two peaks. Ideal general spectrum shown with integration.
13.11 Spin-Spin Splitting in $^1H^1H$ NMR Spectra

13.11 Exercises

Questions

Q13.11.1

Predict the splitting patterns of the following molecules:

A) $\text{Br} \quad$ B) $\text{Br} \quad$ C) $\text{O}$

Q13.11.2

Draw the following according to the criteria given.

A. $\text{C}_3\text{H}_8\text{O}$; two triplet, 1 doublet

B. $\text{C}_4\text{H}_8\text{O}_2$; three singlets

C. $\text{C}_5\text{H}_12$; one singlet

Q13.11.3

The following spectrum is for $\text{C}_3\text{H}_8\text{O}$. Determine the structure.
A triplet; B singlet; C sextet; D triplet

Source: SDBSWeb: http://sdbs.db.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 3 December 2016)

**Solutions**

**S13.11.1**

A. H: Doublet. H: Septet

B. H: Doublet, H: Triplet

C. H: Singlet, H: Quartet, H: Triplet

**S13.11.2**
These are just some drawings, more may be possible.

S13.11.3

Propane

13.12 More Complex Spin-Spin Splitting Patterns

13.12 Exercises

Questions

Q13.12.1

In the following molecule, the C2 is coupled with both the vinyl, C1, and the alkyl C3. Draw the splitting tree diagram.

Solutions

S13.12.1
13.13 Uses of 1H 1H NMR Spectroscopy

13.13 Exercises

Questions

Q13.13.1

How can H 1 1 H NMR determine products? For example, how can you tell the difference between the products of this reaction?

\[ \text{HCl} \rightarrow \text{Cl} \text{ or } \text{Cl} \]

Solutions

S13.13.1

Yes, you are able to determine the difference in the spectra. For the 2-chloro compound will have multiple quartets while the 1-chloro compound will only have a quintet and a triplet for the signals in the ring.

13.6 DEPT 13C 13C NMR Spectroscopy