Question #1
Using the equation shown below, determine the value in ppm of:

- A peak at 800 Hz in a 500 MHz NMR spectrometer
- A peak at 320 Hz in a 200 MHz NMR spectrometer
- A peak at 96 Hz in a 60 MHz spectrometer
- Therefore, why do we measure our x-axis scale in ppm?

\[
\text{chemical shift (in ppm)} = \frac{(10^6) \times \text{chemical shift in Hz}}{\text{spectrometer frequency (in Hz)}}
\]

Question #2
For the molecules listed below, how many chemically (or magnetically) unique HYDROGEN atoms are present in each? How many distinct peak regions would you observe in the proton NMR spectrum? Where would you expect each peak cluster to show up (give estimated chemical shift values) in the proton NMR? You can use Table 15.4 and Figures 15.27, 15.28, 15.29, and 15.31 from the Jones text to help you decide on reasonable shift values. You can also look in the “SAM” booklet.

![Chemical structures](image)

Question #3
For the molecules listed in question #2, what would be the relative integral value for each discernable peak cluster?

Question #4
For the molecules listed in question #2, determine the likely splitting pattern for each unique peak region in its $^1$H-NMR spectrum. You may want to consult Section 15.7 of your Jones text.

Question #5
For the molecules listed in question #2, identify any diagnostic peaks you would observe in each IR spectrum.
Question #6
For the molecules listed in question #2, how many chemically (or magnetically) unique CARBON atoms are present in each? How many distinct peak regions would you observe in the carbon NMR spectrum? Where would you expect each CARBON type to show up (give estimated chemical shift values) in the carbon NMR? You can use Table 15.5 from the Jones text to help you decide on reasonable shift values. You may also consult the “SAM” booklet. In a standard proton-decoupled carbon NMR spectrum, we do not evaluate integral or splitting patterns and all peaks show up as singlets.

Question #7
The following $^1$HNMR spectrum of a C$_{10}$H$_{12}$O$_2$ compound was obtained on a 90 MHz spectrometer.

(a) Ignoring the TMS signal at $\delta = 0$, how many discrete groups of proton signals are present in this spectrum?
(b) What is the multiplicity (s, d, t, q) of the highest field signal from this sample?
(c) The sample has a singlet at $\delta = 3.8$ ppm. In units of Hertz (Hz) how far is this signal from the TMS signal?
(d) What structural feature is suggested by the singlet at $\delta = 3.8$ ppm? Choose among the following:
(e) From multiplet line separations (Js), which of the other signals is coupled to the quartet at $\delta = 2.9$ ppm?
   A $\delta = 1.2$ ppm  B $\delta = 3.8$ ppm  C $\delta = 6.9$ ppm  D $\delta = 7.9$ ppm
(f) Using the integrator trace and the formula of the sample, assign a whole number ratio to the sample signals as follows:
   7.9 ppm signal
   6.9 ppm signal
   3.8 ppm signal
   2.9 ppm signal
   1.2 ppm signal
(g) Which of the following structures best fits the above $^1$HNMR spectrum?
Question #8
Each of the \(^1\)H-NMR spectra (shown below) corresponds to one possible constitutional isomer with a molecular formula of C\(_7\)H\(_{14}\)O. Which isomer produces each spectrum?

The isomers are shown as follows:

- \(\text{CH}_3\text{COCH}_3\)
- \(\text{CH}_3\text{CH}_2\text{COCH}_3\)
- \(\text{CH}_3\text{CH}_2\text{CH}_2\text{COCH}_3\)
- \(\text{CH}_3\text{CH_2CH_2CH_2CH_2COCH}_3\)
- \(\text{CH}_3\text{CH_2CH_2CH_2CH_2CH_2COCH}_3\)
- \(\text{CH}_3\text{CH_2CH_2CH_2CH_2CH_2CH_2COCH}_3\)

The spectra are labeled as follows:

- a.
- b.
- c.
Question #9
Match each IR spectrum with one of the various structures shown below.