Exam 2: CHEM/BCMB 4190/6190/8189 (146 points) Thursday, 30 September, 2021

1). In the example (right), the effect of a 90° (π/2) pulse applied along the "*x*" axis (90° *x*) is shown for a bulk magnetization vector (M_0) at equilibrium (on the '*z*' axis). For 'b', 'c', 'd' and 'e' below, show the effects of the indicated pulses by drawing the missing (originating or resulting) vectors on the coordinate axes. For 'a' and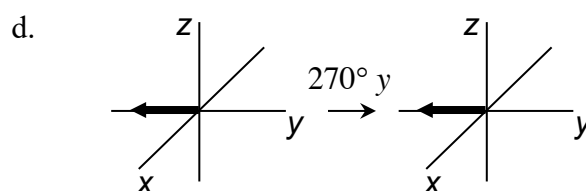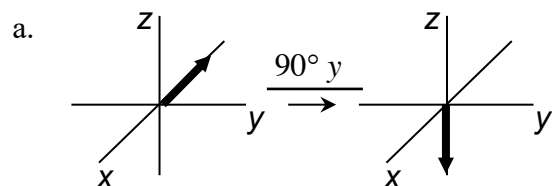 'f', fill in the blank with the correct pulse (angle and axis along which it is applied) that will promote the indicated movement of the bulk magnetization vector. For 'f', first consider the effect of the first pulse, then fill in the blank with the correct second pulse that gives the correct final result. There may be more than one correct answer for some. **(12 points)**

a.

b.

c.

d.

e.

f.
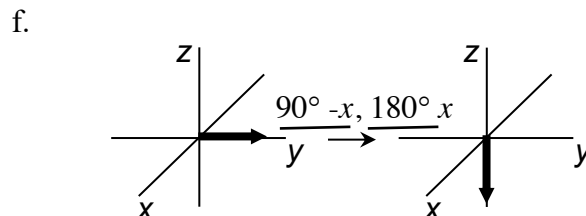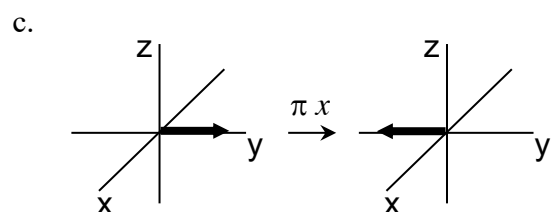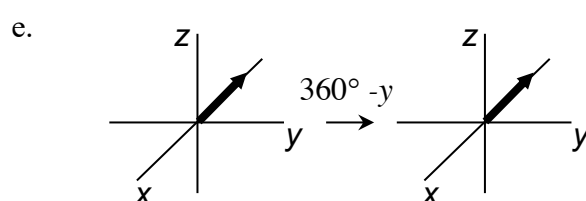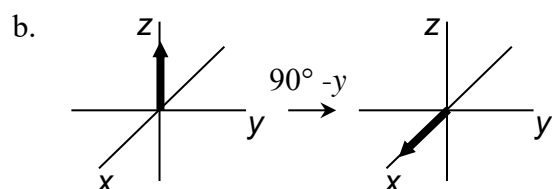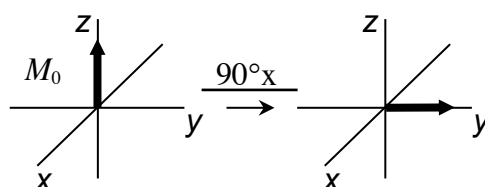
2). For monosubstituted benzene molecules of the type shown at the right, the chemical shifts at the ortho, meta, and para positions can be calculated by the following simple empirical relationship: $\delta^1H = 7.27 + \delta_{corr}$, where δ_{corr} is an empirical correction factor from a table, and is specific for the ortho (δ_{ortho}), meta (δ_{meta}), or para (δ_{para}) position. For instance, when R = -OCOCH$_3$, $\delta^1H_{para} = 7.27 + (\delta_{para}) = 7.27 + (-0.13) = 7.14$ ppm. For R = -COR and R = -NH$_2$, the entries for δ_{ortho}, δ_{meta}, and δ_{para} are missing from the table below. The numerical values for these entries are, from smallest to largest, -0.75, -0.65, -0.25, 0.14, 0.21, and 0.62. Your job is to put these numbers in their correct places in the table. In order to receive credit, you will have to a). draw appropriate resonance structures to justify your table entries, and b). discuss why certain positions are more/less shielded relative to others. **(16 pts)**
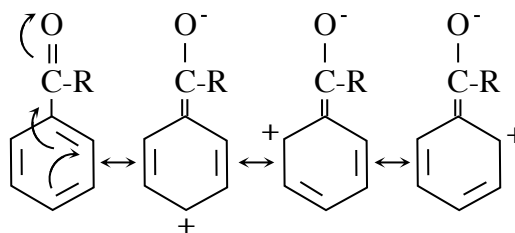
R
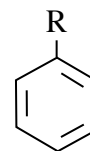
R	δ_{corr}		
	δ_{ortho}	δ_{meta}	δ_{para}
-COR	*0.62*	*0.14*	*0.21*
-NH$_2$	*-0.75*	*-0.25*	*-0.65*
-OCOCH$_3$	-0.25	0.03	-0.13

For R = -COR:
$\delta^1H_{ortho} = 7.27 + (\delta_{ortho}) = 7.27 + (0.62) = 7.89$ ppm
$\delta^1H_{meta} = 7.27 + (\delta_{meta}) = 7.27 + (0.14) = 7.41$ ppm
$\delta^1H_{para} = 7.27 + (\delta_{para}) = 7.27 + (0.21) = 7.48$ ppm

Resonance structures show that ortho and para positions will be deshielded, thus the chemical shifts will be highest in these positions. The chemical shift will be highest at ortho due to proximity to the electron withdrawing substituent.

For R = -NH$_2$
$\delta^1H_{ortho} = 7.27 + (\delta_{ortho}) = 7.27 + (-0.75) = 6.52$ ppm
$\delta^1H_{meta} = 7.27 + (\delta_{meta}) = 7.27 + (-0.25) = 7.02$ ppm
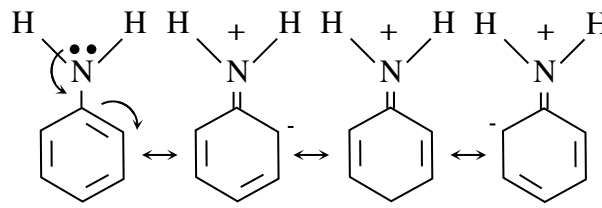$\delta^1H_{para} = 7.27 + (\delta_{para}) = 7.27 + (-0.65) = 6.62$ ppm

Resonance structures show that ortho and para positions will be shielded, thus the chemical shifts will be smallest in these positions. The chemical shift will be smallest at ortho due to proximity to the electron donating substituent.

3). The two chair conformers of hexa-deuteroiodocyclohexane are shown (right). In these structures, the deuterium (^{2}H) atoms are represented by 'D'. The ^{1}H NMR spectrum of this compound was acquired, with broadband decoupling of deuterium, at very low temperature.
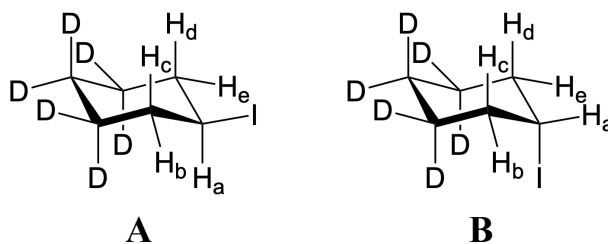
a). *In general*, why might it be advantageous, in some cases, to acquire NMR spectra at low temperature. (**2 points**)

> *In general, the sensitivity of an NMR experiment, as judged by the magnitude of the voltage (emf, ε) induced in the receiver coil, is inversely dependent on temperature, according to the following equation:*

$$\varepsilon = \mathrm{dM/dt} = \gamma M_0 B_0 = \frac{N\gamma^3 \hbar^2 B_0^2 I(I+1)}{3k_B T}$$

> *Therefore, in general, under some circumstances, an increase in sensitivity could be expected when NMR spectra are recorded at lower temperatures.*

b). For compounds such as cyclohexane derivatives, why might it be advantageous, under some circumstances, to acquire the spectra at very low temperature. (**4 points**)

> *For such cyclohexane derivatives, when there are no bulky substituents, the energetic barrier to chair-chair interconversion is very low, resulting in very fast interconversion of the chair conformers. In such a case, the NMR spectrum will be the average spectrum of the forms present, weighted by the equilibrium percentages of each. If it is necessary or desirable to record spectra of the individual conformers, lowering the temperature can increase the energetic barrier to interconversion to the point that interconversion is slowed significantly. If the interconversion is very slow (if the lifetimes of the individual conformers are long enough), then signals in the spectrum corresponding to each of the conformers can be observed.*

c). In a ^{1}H NMR spectrum of only conformer 'A' of hexa-deuteroiodocyclohexane, how many signals would you expect to see? Likewise, in a ^{1}H NMR spectrum of only conformer 'B' of hexa-deuteroiodocyclohexane, how many signals would you expect to see? You will have to justify your answers for credit. (**6 points**)

> *For both conformers there is a plane of symmetry that includes the carbon atom bearing the iodine atom (which we will designate as carbon '1'), the iodine atom, hydrogen Ha, carbon atom '4' and the deuterium atoms on carbon '4' (all circled with dashed line, below left).*
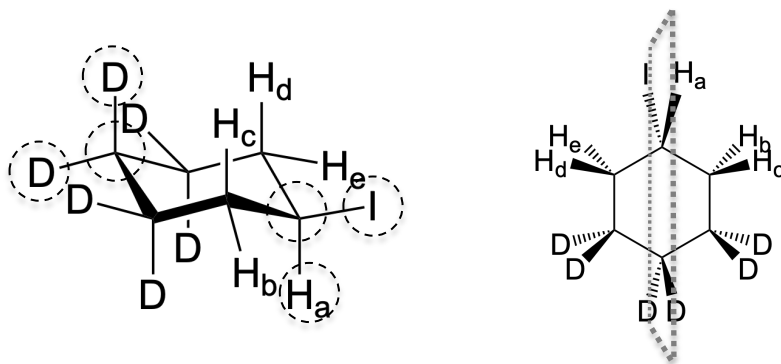

> *Therefore, hydrogens Hc and Hd are in mirror image chemical environments (entiotopic), so they have the same chemical shift and will give one signal. Likewise, hydrogens Hb and He are also in mirror image chemical environments (enantiotopic), and they will give a single signal. Finally, Ha will give a signal. So, for each conformer, there will be a total of 3 signals in the ^{1}H spectrum of that conformer.*

d). In a ^{13}C NMR spectrum of only conformer 'A' of hexa-deuteroiodocyclohexane, how many signals would you expect to see? Likewise, in a ^{13}C NMR spectrum of only conformer 'B' of hexa-deuteroiodocyclohexane, how many signals would you expect to see? You will have to justify your answers for credit. (**6 points**)

> *As indicated in the answer to part 'c', there is a plane of symmetry as shown. There will be a signal from the carbon atom bearing the iodine atom (carbon '1'), and there will be a signal from the carbon atom at position '4'. The carbon atoms at positions '2' and '6' are in mirror image environments (enantiotopic), so they will give a single signal. Likewise, this is the case for the carbon atoms at positions '3' and '5'. So, there will be 4 signals in the ^{13}C spectrum of either of the conformers.*

e). In the ^{1}H NMR spectrum of hexa-deuteroiodocyclohexane, acquired with broadband decoupling of deuterium, at very low temperature using a 400 MHz magnet, the signals below are from hydrogen 'Ha'.

A   **B**
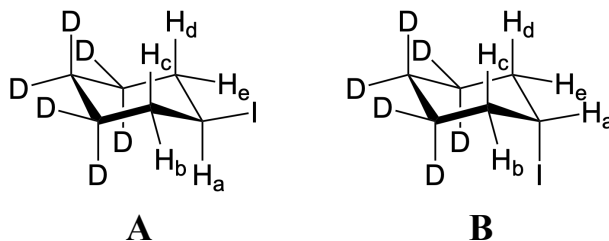
Which conformer, '**A**' or '**B**', gives the signal below on the left for 'Ha', and which gives the signal below on the right for 'Ha'? You will have to provide a strong justification for credit. As part of this justification, you will have to determine the values of the coupling constants in each signal and assign them to the correct coupled ^{1}H nuclei. You also will have to describe the multiplicity of each signal and why that particular multiplicity is observed, based on the structure and the coupling constants. (**8 points**)
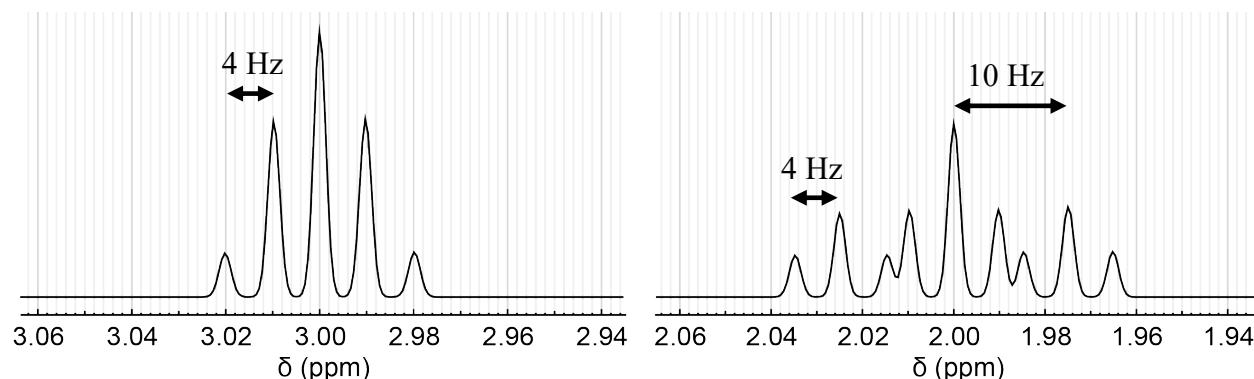
For both conformers, there is a plane of symmetry (see answer to part 'c') such that 'Hb' and 'He' have the same chemical shift (enantiotopic), and 'Hc' and 'Hd' also have the same chemical shift (enantiotopic). Therefore, for both conformers, the signal from 'Ha' would be split (n=2, n+1=3) into a triplet by 'Hb'/'He', and then into another triplet by 'Hc'/'Hd'. So, in both cases, the expected multiplet would be a triplet of triplets.

*However, for conformer '**B**', because 'Ha' is equatorial, all of the dihedral angles to the other hydrogens are about 60° (both equatorial-equatorial, and equatorial-axial), so, according to the Karplus relationship, the coupling constants between 'Ha' and each of the other hydrogens would be expected to be small and about the same magnitude (4-5 Hz). Because of this, the components of the triplet of triplets would tend to overlap in such a way as to resemble a quintet (n=4, n+1=5). <u>The signal on the left, then, can be assigned to conformer '**B**'</u>. This is consistent with the single coupling constant that can be measured, which is 4 Hz. So, the coupling constant from Ha to each of the other hydrogens is about 4 Hz.*

*For conformer '**A**', the 'Ha' hydrogen is axial. Therefore, the dihedral angle between 'Ha' and 'Hc'/'Hd' (axial-axial) is about 180°. According to the Karplus relationship, the coupling constant should therefore be large (10-12 Hz). The dihedral angle between 'Ha' and 'Hb'/'Hd' (axial-equatorial) is about 60°, so that coupling constant would be small (4-5 Hz). So, the multiplet structure could be expected to resemble the predicted triplet of triplets. <u>That is what is observed for the signal on the right, so this can be assigned to the '**A**' conformer</u>. This is consistent with the observed coupling constants measured in the multiplet (4 Hz and 10 Hz).*

4). In a magnetic field (600 MHz), the energy difference between the lowest and highest energy states for a particular nucleus ($\gamma = 2.00 \times 10^7$ rad T^{-1} s^{-1}) is 2.080×10^{-25} J. What is the spin angular momentum quantum number, I, for this nucleus? You will have to show your work and explain your answer for credit. **(6 points)**

The energy between any two adjacent energy levels is:

$$E = \gamma\hbar B_0$$

There are (2I+1) levels, ranging from I to -I (I, I-1, I-2…..-I). So, the highest and lowest values of I are separated by 2I (I-(-I) = 2I). So, the energy between the highest and lowest energy levels is then:

$$E = (2I)\gamma\hbar B_0$$

$$E = (2I)\gamma\hbar B_0 \quad I = \frac{E}{2\gamma\hbar B_0} = \frac{2.080 \times 10^{-25}\text{J}}{2.00 \times 10^7 \text{ rad T}^{-1}\text{s}^{-1} \frac{6.626 \times 10^{-34} \text{ J s}}{\pi} \, 14.09 \text{ T}} = 3.5 = \frac{7}{2}$$

5). How many signals will there be in ^{13}C NMR spectra of each of the following compounds? You will have to justify your reasoning in each case for credit. (**12 points**)

A
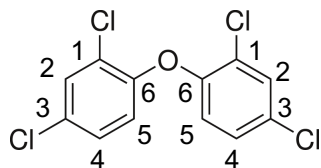
B
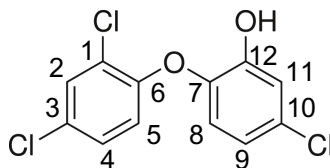
C
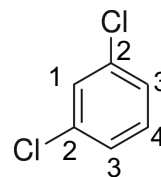
D
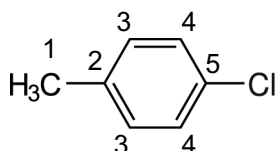
E
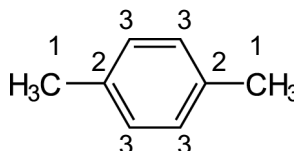
F
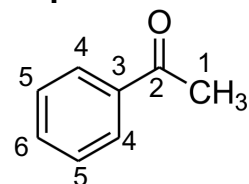
For each of the molecules, the equivalent positions are indicated in the figure using integers, with equivalent positions indicated by equal integers. In each case, these are related by a symmetry operation, resulting in chemical equivalence. For molecule 'A', therefore, we would predict six signals in the ^{13}C NMR spectrum. Likewise, for 'B', 'C', 'D', 'E', and 'F', we would expect twelve, four, five, three and six signals, respectively.

6). The following questions regarding the molecule oxetane (right).

a. Are the hydrogens labeled 'a' homotopic, enantiotopic, or diastereotopic? (**2 points**)

enantiotopic
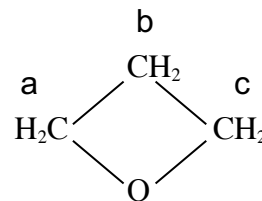
b. Are the hydrogens labeled 'b' homotopic, enantiotopic, or diastereotopic? (**2 points**)

homotopic

c. Will the hydrogens labeled 'c' always have the same chemical shift? You will have to explain for credit. (**4 points**)

No. These hydrogens are enantiotopic. Enantiopic hydrogens are not in chemically identical environments, but mirror image chemical environments. In normal solvents, they will have identical chemical shifts, but in chiral solvents, if they interact with the solvent, the chemical shifts may not be equivalent.

d. Sketch the signals that would appear in the ^{1}H NMR spectrum of oxetane in CDCl$_3$. Clearly indicate which hydrogens give rise to each signal. For each multiplet, indicate the expected relative intensities of the individual peaks in that multiplet. For credit you will have to explain in detail your signals/answers. (**6 points**)

The hydrogens on the methylene groups bound to the oxygen will all have the same chemical shift. Each pair (the 'a' pair and the 'c' pair) are enantiotopic, and will have the same chemical shifts in achiral environments. Furthermore, there is a plane of symmetry through the carbon and oxygen atoms so the hydrogens on 'a' are chemically equivalent to those on 'c'. The signal from them will be a downfield-shifted (because of the electronegative oxygen) triplet (split by the hydrogens of the methylene group not bound to the oxygen, intensities 1:2:1). The hydrogens on the methylene group not bound to the oxygen are homotopic and chemically equivalent, and are split by the 4 (equivalent) hydrogens of the neighboring methylene groups into a more upfield-shifted quintet (intensities 1:4:6:4:1).
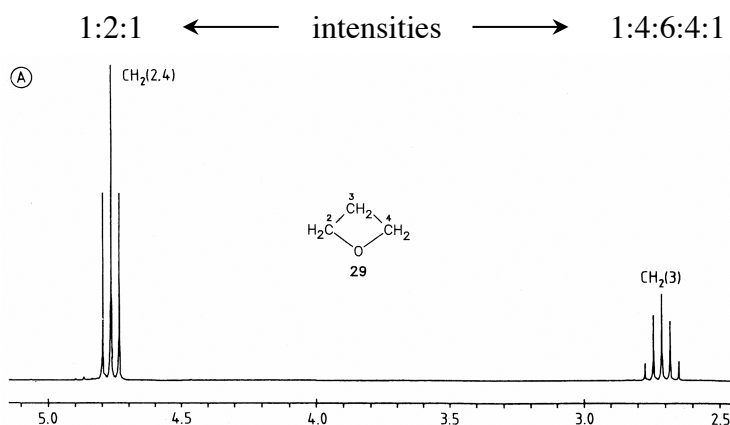
7). The ^1H NMR spectra (right) show the signals from two hydrogens on adjacent carbon atoms that are coupled (^3J) to one another. From top to bottom, the spectra clearly demonstrate the spectral changes that occur when the difference between the Larmor frequencies of the two hydrogens decreases. The spin system designations (AX, AB, A$_2$) are shown. A space is provided for the A$_2$ spectrum but the spectrum is not shown.

$\Delta v/J$

−CH−CH−

20 — AX

14

7 — AB

1.5

0 — A$_2$
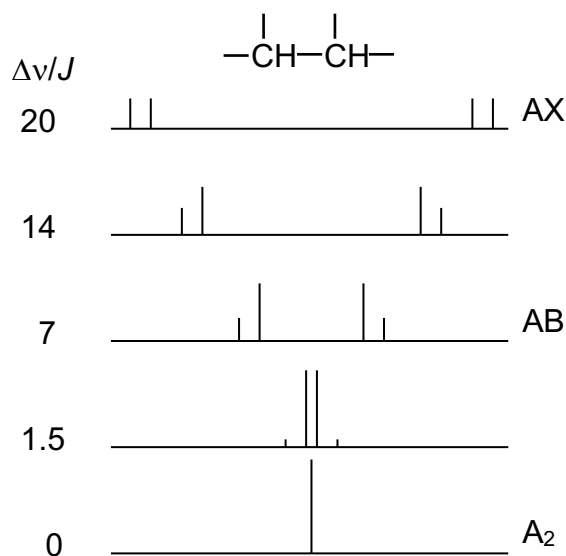
a. What are 'AX' and 'AB' spin systems? (**4 points**)

> *AX spin systems are those for which the difference between the Larmor frequencies of the two coupled nuclei is much larger than the coupling constant, J (first order). In AB systems, this difference is on the same order as J (second order).*

b. Draw the expected A$_2$ spectrum in the space provided above. Provide an explanation/justification for your answer. Your explanation (and drawing) should include the expected intensity of the signals/peaks in the A$_2$ system relative to the intensities of the peaks in the AX system. (**6 points**).

> *When the resonance frequencies are identical ($\Delta v = 0$) for two coupled hydrogens, they give rise to a single signal. This is clear from the progression shown above as Δv approaches zero: the intensities of the outer components of the doublets decrease in intensity as the inner components increase. At the limit ($\Delta v = 0$), only a singlet remains. This relative intensity of this singlet would be four times as large as the intensities of the individual peaks in the AX system ($\Delta v = 20$) shown, as these four peaks collapse into one.*

c. What word or term in NMR spectroscopy is also used to describe nuclei that comprise A$_2$ systems? Please explain. (**4 points**)

> *The term "equivalent" can be used to define or describe two coupled hydrogens with identical chemical shifts.*

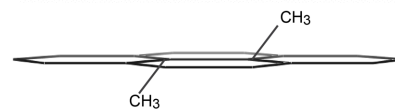**8**). The chemical shifts of the hydrogen nuclei in benzene are 7.28 ppm. *Estimate* the chemical shifts for the equivalent hydrogens of the methyl groups in the dimethylpyrene compound shown (right). *To receive credit you will have to provide a good justification for your estimate.* (**4 points**)
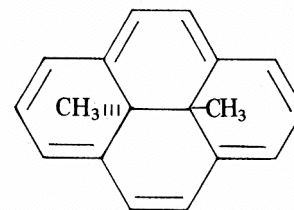
The magnetic anisotropy of the π electron ring currents in benzene results in deshielding hydrogens in the plane of the ring (hence, the chemical shift of 7.28 ppm) and shielding hydrogens and other nuclei above and below the plane. This is true of most all flat planar aromatic systems, such as the dimethylpyrene molecule shown. Therefore, one would expect that the chemical shifts for the methyl hydrogens would be shielded relative to methyl groups in alkanes. This is the case here, as the chemical shifts of the hydrogens in the methyl groups of the dimethyl pyrene molecule shown are approximately -4.2 ppm.

9). The ^{1}H NMR chemical shifts (ppm) for the hydrogen nuclei in the indicated (circled) methyl groups in pinane and α- and β-pinene are shown below. Provide an explanation for the variation of these methyl (circled) ^{1}H chemical shifts between pinane, α-pinene, and β-pinene. (**6 points**)
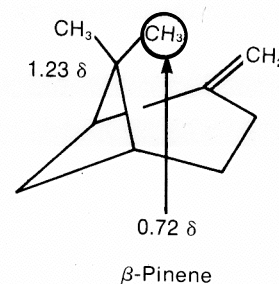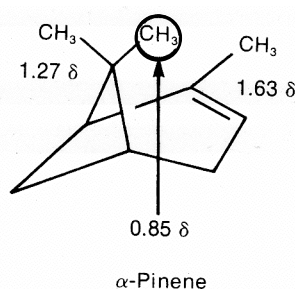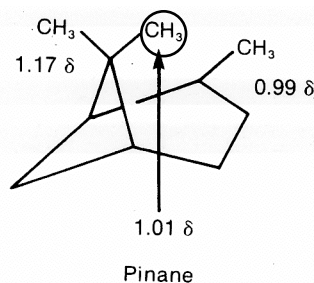
In the pinene molecules, the methyl group in question is positioned near the double bond and along its length in both molecules. Given the trend, one might expect that the shielding, relative to pinane, is the result of the magnetic anisotropy of the double bond, and that the methyl group is in the shielding region. This is the case.

10). Please explain what "shielding" means with respect to NMR. Please use complete sentences and avoid using symbols, equations and drawings. Your explanation should address the relationship between shielding and resonance frequency. (**6 points**)

> *Electron currents are induced in the electron shells surrounding nuclei in the presence of a static magnetic field. These currents produce magnetic fields that oppose or augment the main field, depending on the nature of the atom, the symmetry of the charge distribution, and other factors. Thus, the effective magnetic field experienced by a given nucleus is mediated by this electron shielding. Because resonance frequency is dependent linearly on the static magnetic field strength, shielding governs the observed resonance frequencies of nuclei. A nucleus that precesses with a low frequency ("upfield" shift) is said to be highly shielded, and one that precesses at a higher frequency ("downfield" shift) is said to be highly deshielded.*

11). For a sample of $CHCl_3$, you apply a very long (seconds), low power pulse at the ^1H frequency of the single ^1H nucleus in the molecule. Immediately after this pulse, you apply a normal, high power 90 degree pulse at the same frequency and then record the FID. Sketch what you would expect the FID to look like. Also, sketch the spectrum you would expect to observe following Fourier transformation of the FID. You must thoroughly explain your answers for credit. (**6 points**).

> *A long pulse leads to equilibration of the α and β spin populations of the nucleus. In such an instance, there is no net, bulk (macroscopic) magnetization in either the longitudinal direction or transverse plane. If some longitudinal component were present, the 90 degree pulse would rotate that component into the transverse plane and it could then be detected. Because there is no such component, the 90 degree pulse does nothing, and there is no detectible signal. So, the FID will just be noise, and there will be no observable signals in the transformed spectrum.*

12). Circle the word in each pair of parentheses that makes the following statement true: As the value for the shielding constant, σ, decreases, this indicates (decreased/ increased) shielding of a nucleus, a/an (decrease increase) in the effective magnetic field experienced by the nucleus, a/an (downfield/ upfield) shift in the chemical shift, and a (lower higher) resonance frequency for the nucleus. (**4 points**)

13). For ethyl phenylacetate, the regions from ~ 0-90 ppm of the ^{1}H-coupled (top) and ^{1}H-decoupled (bottom) ^{13}C NMR spectrum are shown (right). The pulse sequence used to record the decoupled spectrum on natural isotopic abundance phenylacetate is shown below.

broadband or "cpd" sequence
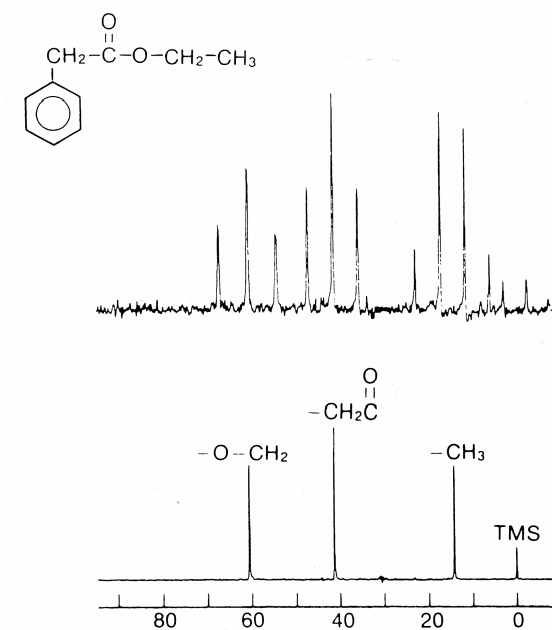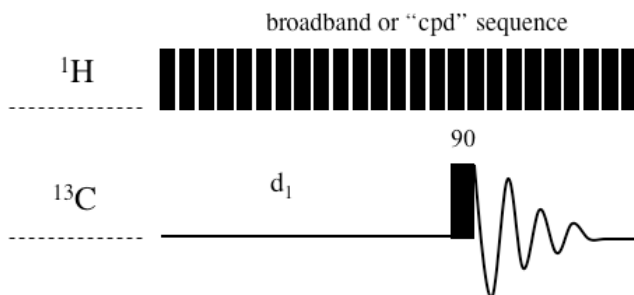
Sketch the simple ^{1}H NMR spectrum of the -O-CH$_2$-CH$_3$ group of ethyl phenylacetate. Then sketch the ^{1}H NMR spectrum that you would observe if you recorded the ^{1}H spectrum of natural isotopic abundance phenylacetate with ^{13}C broadband decoupling (pulse sequence shown at right). You will have to explain the appearance of each signal in the spectra, and the differences observed when using the decoupling sequence. (**4 points**)

broadband or "cpd" sequence
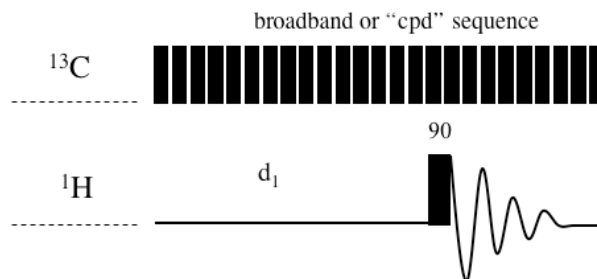
The ^{1}H spectrum will be comprised of two signals, one (downfield, perhaps ~ 3 ppm) will be a quartet, corresponding to the -CH$_2$- group split by the three hydrogens of the -CH$_3$ group, and the other will be upfield (perhaps 1-2 ppm) and will be a triplet, due to the -CH$_3$ group split by the two -CH$_2$- hydrogens. The integral of the downfield peak will be 2, and that of the upfield peak will be 3.
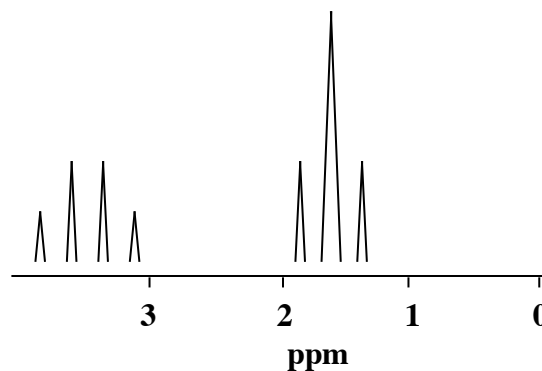
The spectrum will not noticeably change when broadband ^{13}C decoupling is applied, as ~99% of the carbon atoms to which the ^{1}H nuclei are bound are ^{12}C.

14). Shown (right) are two ^{13}C spectra of the compound shown. One was acquired with broadband ^{1}H-decoupling, and the other with gated ^{1}H-decoupling. The signal at 78 ppm is due to solvent.
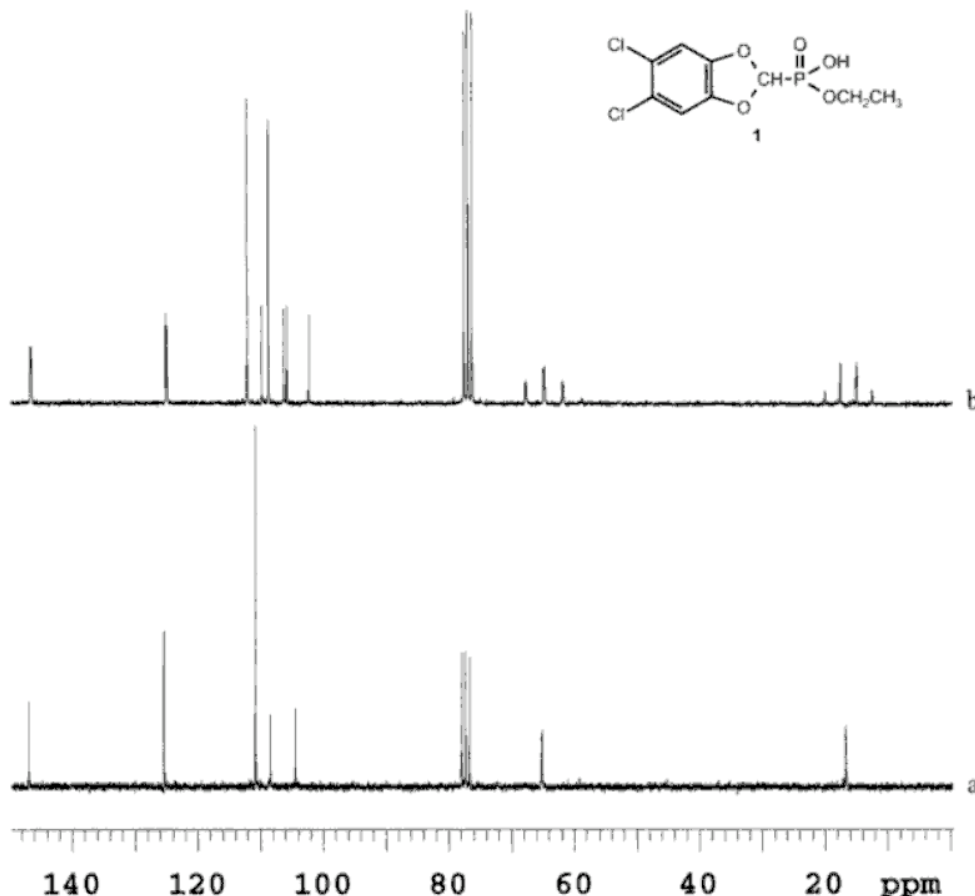
a. Which spectrum was acquired with broadband ^{1}H-decoupling and which was acquired with gated broadband ^{1}H-decoupling. You must explain your reasoning for credit. (**4 points**)

> *Broadband ^{1}H decoupling removes splitting of signals in ^{13}C spectra due to attached hydrogens. Gated broadband decoupling does not. Therefore, the spectrum in 'a' is the broadband decoupled spectrum, and 'b' is the gated decoupled spectrum.*

b. Given the signal-to-noise of each spectrum, what can you conclude about the differences between acquisition parameters for these two spectra? You must explain your reasoning for credit. (**4 points**)

> *If the acquisition parameters were identical, the signal-to-noise of the broadband decoupled spectrum would be substantially better than the gated experiment, because both multiplet collapse and the nuclear Overhauser effect would lead to high sensitivity. However, the signal-to-noise of 'b' above (gated) is significantly better than 'a' (broadband). This leads to the conclusion that acquisition parameters were not the same. Most likely the spectrum in 'b' was acquired with more scans, or, perhaps, with a longer d_1 time period to increase the sensitivity enhancement due to the NOE.*

15). The ^{13}C NMR spectrum (right, bottom) shows the ^{13}C-^{1}H doublet from a methine group in the molecule CHX$_3$, where 'X' are halides (i.e., chloroform). The spectrum at the top shows the results of selective, on-resonance, decoupling of ^{1}H from ^{13}C in this molecule. This is done with the pulse sequence below with the decoupler frequency matching the Larmor frequency of the ^{1}H in the molecule. As a result, the ^{13}C signal is decoupled from the ^{1}H and appears as a singlet. The spectrum in the center (right) is the result of off-resonance decoupling of ^{1}H, where the decoupler frequency is not at the Larmor frequency of the ^{1}H. The multiplet has partially collapsed (the apparent coupling constant is smaller than the actual value).

^{1}H

90

^{13}C d_1

200 100 0 -100 -200   Hz
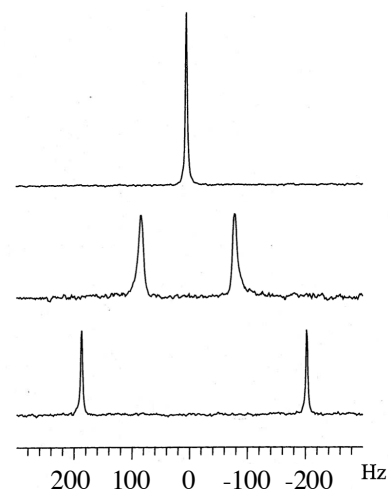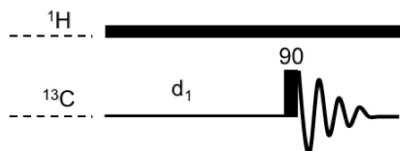
a. What determines the difference between the actual and observed coupling constants (in Hz) in an off-resonance decoupling experiment such as the one described for the spectrum above? (**4 points**)

The difference between the actual and observed coupling constant, or the decrease in the coupling constant as a result of the off-resonance decoupling, is dependent on the strength of the decoupler field (B_2), and the frequency difference between the Larmor frequency of the ^{1}H nucleus of interest and the frequency at which the decoupling field is applied (Δv). The equation below describes the relationship, where J is the actual ^{13}C-^{1}H coupling constant and J_r is the reduced (observed) coupling constant resulting from the off-resonance decoupling.

$$B_2 = \frac{\Delta v \sqrt{J^2 - J_r^2}}{J_r} \approx \frac{J \Delta v}{J_r}$$

b. Calculate the difference between the Larmor frequency of the ^{1}H in the molecule and the frequency at which the decoupling field is applied for the off-resonance experiment shown above if the decoupler field strength (B_2) used is 10 kHz. (**4 points**)

From the spectra above, we can estimate the actual coupling (J) as 400 Hz, and we can estimate the reduced coupling (J_r, observed coupling in the off-resonance experiment) to be 160 Hz.

$$\Delta v = \frac{B_2 \times J_r}{\sqrt{J^2 - J_r^2}} = \frac{10,000 \text{ Hz} \times 160 \text{ Hz}}{\sqrt{400^2 - 160^2} \text{ Hz}} = \frac{1.6 \times 10^6 \text{ Hz}^2}{366.6 \text{ Hz}} = 4364 \text{ Hz}$$

$$\Delta v \approx \frac{B_2 \times J_r}{J} = \frac{10,000 \text{ Hz} \times 160 \text{ Hz}}{400 \text{ Hz}} = \frac{1.6 \times 10^6 \text{ Hz}^2}{400 \text{ Hz}} = 4000 \text{ Hz}$$

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You may find some of the information below useful:

Table 1-1.
Properties of some nuclides of importance in NMR spectroscopy.

Nuclide	Spin I	Electric quadrupole moment[a] $[eQ]$ $[10^{-28}\ m^2]$	Natural abundance) [%]	Relative sensitivity[b]	Gyromagnetic ratio γ[a] $[10^7\ rad\ T^{-1}\ s^{-1}]$	NMR frequency [MHz][b] $(B_0 = 2.3488\ T)$
^1H	1/2	–	99.985	1.00	26.7519	100.0
^2H	1	2.87×10^{-3}	0.015	9.65×10^3	4.1066	15.351
^3H[c]	1/2	–	–	1.21	28.5350	106.664
^6Li	1	-6.4×10^{-4}	7.42	8.5×10^{-3}	3.9371	14.716
^{10}B	3	8.5×10^{-2}	19.58	1.99×10^{-2}	2.8747	10.746
^{11}B	3/2	4.1×10^{-2}	80.42	0.17	8.5847	32.084
^{12}C	0	–	98.9	–	–	–
^{13}C	1/2	–	1.108	1.59×10^{-2}	6.7283	25.144
^{14}N	1	1.67×10^{-2}	99.63	1.01×10^{-3}	1.9338	7.224
^{15}N	1/2	–	0.37	1.04×10^{-3}	–2.7126	10.133
^{16}O	0	–	99.96	–	–	–
^{17}O	5/2	-2.6×10^{-2}	0.037	2.91×10^{-2}	–3.6280	13.557
^{19}F	1/2	–	100	0.83	25.1815	94.077
^{23}Na	3/2	0.1	100	9.25×10^{-2}	7.0704	26.451
^{25}Mg	5/2	0.22	10.13	2.67×10^{-3}	–1.6389	6.1195
^{29}Si	1/2	–	4.70	7.84×10^{-3}	–5.3190	19.865
^{31}P	1/2	–	100	6.63×10^{-2}	10.8394	40.481
^{39}K	3/2	5.5×10^{-2}	93.1	5.08×10^{-4}	1.2499	4.667
^{43}Ca	7/2	-5.0×10^{-2}	0.145	6.40×10^{-3}	–1.8028	6.728
^{57}Fe	1/2	–	2.19	3.37×10^{-5}	0.8687	3.231
^{59}Co	7/2	0.42	100	0.28	6.3015	23.614
^{119}Sn	1/2	–	8.58	5.18×10^{-2}	–10.0318	37.272
^{133}Cs	7/2	-3.0×10^{-3}	100	4.74×10^{-2}	3.5339	13.117
^{195}Pt	1/2	–	33.8	9.94×10^{-3}	5.8383	21.499

B_0 (Tesla, T)	Resonance frequencies (MHz)	
	^1H	^{13}C
9.4	400	100.6
11.74	500	125.7
14.09	600	150.9
18.79	800	201.2

$\gamma_{1H} = 26.7519 \times 10^7$ rad/T/s, $I = 1/2$ $\gamma_{13C} = 6.7283 \times 10^7$ rad/T/s, $I = 1/2$
$\gamma_{10B} = 2.8747 \times 10^7$ rad/T/s, $I = 3$ $\gamma_{15N} = -2.7126 \times 10^7$ rad/T/s, $I = 1/2$
$\gamma_{11B} = 8.5847 \times 10^7$ rad/T/s, $I = 3/2$ $\gamma_{17O} = -3.6280 \times 10^7$ rad/T/s, $I = 5/2$

You may find some of the following information or equations useful:

$k_B = 1.381 \times 10^{-23}$ J/K

Avagadro's number $= 6.02214179 \times 10^{23}$ mol^{-1}

$h = 6.626 \times 10^{-34}$ Js

$\hbar = h/(2\pi)$

$P = \hbar\sqrt{I(I+1)}$

$P_Z = m\hbar$

$\mu = \gamma P = \hbar\gamma\sqrt{I(I+1)}$

for $m = \dfrac{1}{2}$, $\cos(\theta) = \dfrac{m\hbar}{\hbar\sqrt{I(I+1)}} = \dfrac{m}{\sqrt{I(I+1)}}$

$\pi/2$ radians $= 90°$

$M_0 = \dfrac{N\gamma^2\hbar^2 B_0 I(I+1)}{3k_B T}$

$B_2 = \dfrac{\Delta v\sqrt{J^2 - J_r^2}}{J_r} = \dfrac{J\Delta v}{J_r}$

$\varepsilon = \dfrac{dM}{dt} = \gamma M_0 B_0 = \dfrac{N\gamma^3\hbar^2 B_0^2 I(I+1)}{3k_B T}$

$\Delta v = v_{BS} - v_0 = \dfrac{B_2^2}{2(\Delta B)} = \dfrac{B_2^2}{2(v_0 - v_i)}$

$S/N \propto NS^{1/2}$ (signal-to-noise improves with (number of scans)$^{1/2}$)

$m = (-I, -I+1, \ldots, I-1, I)$

$E = -\mu_z B_0 = -m\gamma\hbar B_0$

$\Delta E = \mu_z B_0 = \gamma\hbar B_0 = hv_L = hv_1$

$v_L = |\gamma/(2\pi)|\, B_0 = \omega_0/(2\pi)$

$\omega_0 = \gamma B_0$

$\Delta\delta = \dfrac{\Delta v}{\text{observe frequency}} \times 10^6$

$M_y = M_0 e^{-t/T_2^*}$

$M_z = M_0(1 - e^{-t/T_1})$

$M_z = M_0(1 - 2e^{-t/T_1})$

$\Delta v_{1/2} = \dfrac{1}{\pi T_2^*}$

$\dfrac{1}{T_2^*} = \dfrac{\gamma\Delta B_0}{2} + \dfrac{1}{T_2}$ $\dfrac{1}{T_2^*} = \dfrac{1}{T_2} + \dfrac{1}{T_2(B_0)}$

$t_{zero} = T_1\ln(2)$

$\eta = \gamma_a / (2\gamma_x)$

$I = (1 + \eta) I_0$

$I \propto 1/r^6$

$\Theta = \gamma B_1 \tau_p$

$\dfrac{N_\beta}{N_\alpha} \approx 1 - \left(\dfrac{\gamma\hbar B_0}{k_B T}\right)$

$B_{eff} = B_0(1-\sigma)$

$\upsilon_L = \dfrac{\gamma}{2\pi}(1-\sigma)B_0$

SW=1/(2DW)=Nyquist frequency (v_{NQ})/2
AQ=DW*TD
DR=2SW/TD=1/AQ
(TD≡NP)

$\cos\alpha_{Ernst} = e^{-((d_1 + AQ)/T_1)}$

$\pi/2$ radians $= 90°$

$\Delta v \gg J$
$1 + \gamma_A/\gamma_X$ $1 - \gamma_A/\gamma_X$
multiplicity=$2nI + 1$
$\Theta = 2\pi J\tau$