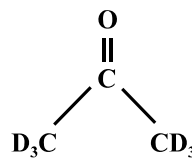**T5a Practice problem** (Refer to pages C58-C61 in the online manual):

1.   sample = d_6-acetone   (Refer to Figures 5-1 and 5-2)

a)   Draw the structure. Show all bonds and atoms explicitly.

b)   Tabulate the ^{13}C nmr data and assign all of the peaks using a diagram of the proposed structure.

| chemical shift, δ (ppm)	multiplicity	coupling constant (Hz)	assignment	coupled to
206.0	*singlet*	-	C_b	-
29.7	*septet*	19	C_a	D
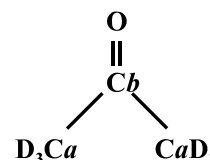
c)   How do you calculate the coupling constant in Hz? Show the calculation in this case. (note: SF = spectrometer frequency on the spectrum)

    Hz   = ppm x spectrometer frequency in MHz
           = 0.307 ppm x 62.896 MHz   note: 0.307 is avg of 6 'gaps' in the septet
           = 19.3 Hz rounded to nearest 1 Hz = 19 Hz

d)   Draw tree diagrams to justify all the observed multiplets. Include relative intensities. *Graph paper is strongly recommended.*

    Notes:
- *because the C_a is split by D (I=1), each 'fork' in your diagram will result in __three__ branches*
- *there are three equivalent D on each C_a so you will need to split the tree three times*
- *careful tracking of the number of lines produced by each split is essential*
- *this will result in a 1:3:6:7:6:3:1 septet*
- *C_b is a singlet as the $^2J(C_bD)$ coupling is very small*
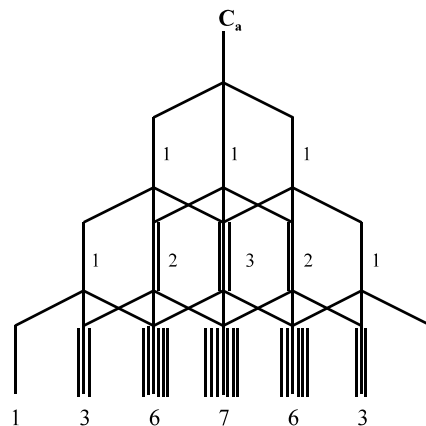
e)   Which band(s) in the IR are diagnostic? What functional group(s) do these bands indicate?
           1705 cm^{-1} C=O str.
           2256 cm^{-1} C-D str.

f)   What would the ^1H nmr show for this sample? Why?
           Nothing - because there are no protons
    OR   δ2.05 s - due to d_5-acetone contamination in d_6-acetone (see manual page D82)

2.   Molecular formula = C_8H_6 (Refer to Figures 5-3 to 5-5)
a)   Calculate the # DBE. Show the calculation.

> ***#H's indicated = 2n + 2 = 2(8) + 2 = 18***
> ***#DBE = (# H's indicated - # H's in formula) ÷ 2***
> ***= (18-6) ÷ 2 = 6 DBE***

b)   Give two suggestions of what this number of DBE could indicate?

> ***benzene ring + two double bonds***
> ***benzene ring + one triple bond***

c)   Which band(s) in the IR are diagnostic? What functional group(s) do these bands
indicate?

> ***3291 cm-1   ≡C-H str.***
> ***and/or 2109 cm⁻¹ C≡C str., conj.***
> ***and/or 757, 691 cm⁻¹ mono sub. benzene ring***

d)   Tabulate the ^{13}C and DEPT-135 nmr data and assign all of the peaks using a diagram of
the proposed structure.

chemical shift, δ (ppm)	DEPT signal	- 135 inference	assignment
132.2	↑	CH or CH_3	C_d or C_e
128.8	↑	CH or CH_3	C_f (by height)
128.3	↑	CH or CH_3	C_e or C_d
122.2	x	C	C_c
83.7	x	C	C_b
77.2	↑	CH or CH_3	C_a
77.1 t	x	-	$CDCl_3$