T4c Practice problem (Refer to pages C46-C47 in the online manual)

Molecular formula = C_8H_8 (Refer to Figures 4-11 to 4-13)

a) Calculate the # DBE, show the calculation. What does this value indicate?

#H's indicated = 2n + 2 = 2(8) + 2 = 18

#DBE = (# H's indicated - # H's in formula) ÷ 2

= (18-8) ÷ 2 = 5 DBE benzene ring + one double bond

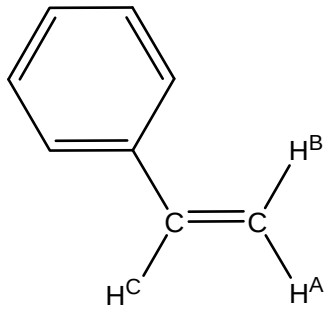
b) Are there any diagnostic IR bands? If so, what functional group(s) do these bands indicate?

991, 908 cm^{-1} (s) =C-H bend, monosub. alkene

776, 697 cm^{-1} (s) =C-H bend, monosub. benzene

c) Tabulate the ^1H nmr data and assign all of the peaks using a diagram of the proposed structure. *Hint: the δ 1.50 signal can be ignored (structurally) as it is due to water in the $CDCl_3$.*

chemical shift, δ (ppm)	multiplicity	coupling constant (Hz)	integration		assignment	coupled to
			actual	relative		
7.45-7.24	*multiple resonances*	*-*	*88.087*	*5 H*	H_{Ar} + $CDCl_3$	*-*
6.75	*doublet of doublets*	*18* *11*	*17.170*	*1 H*	H_C	H_B H_A
5.78	*doublet*	*18*	*18.389*	*1 H*	H_B	H_C
5.27	*doublet*	*11*	*18.710*	*1 H*	H_A	H_C



notes:

- ***H_{Ar} refers to the five aromatic protons on the benzene ring. These are not equivalent, but because the signals can't be differentiated they are lumped together in the assignment.***
- ***Typical coupling constants: geminal (H_AH_B) 0-2 Hz, cis (H_AH_C) 7-10 Hz, trans (H_BH_C) 14-16 Hz. So although H_A does couple to both H_B and H_C, this is not seen in the nmr as the J value is too small. A bigger magnet (ie: 500HMz) would likely show this.***

d) Draw tree diagrams to justify all the observed multiplets. Include relative intensities.