Chem 205 web spectroscopy problem set answers

Circle the letters below corresponding to correct answers

1. 100 ml of a solution contains 0.050 g of a coloured compound that absorbs exactly half the incident light intensity at 500 nm when the solution is in a 1.00 cm wide spectrophotometer cell. The cell width that would absorb 75% of the incident light intensity is:

a. 0.5 cm
b. 1.0 cm
c. 2.0 cm
d. 4.0 cm
e. ($\log_{10} 2$) cm
f. none of the above

ANSWER:

According to Lambert-Beer law absorbances for two different situations can be expressed as:

$$A_1 = -\log\frac{I_1}{I_0} = \varepsilon_{\lambda 1} c_1 l_1$$

$$A_2 = -\log\frac{I_2}{I_0} = \varepsilon_{\lambda 2} c_2 l_2$$

where $\varepsilon_{\lambda 1} = \varepsilon_{\lambda 2} = \varepsilon_{\lambda}$, $c_1 = c_2$,
$I_1 = I_1(\text{transmitted}) = 1 - I_1(\text{absorbed}) = 50\% I_0 = 0.5 I_0$
and $I_2 = I_2(\text{transmitted}) = 1 - I_2(\text{absorbed}) = 25\% I_0 = 0.25 I_0$

$$\frac{A_1}{A_2} = \frac{l_1}{l_2} \Rightarrow \frac{-\log 0.5}{-\log 0.25} = \frac{1cm}{l_2}$$

$$l_2 = 2cm$$

2. The mass of the coloured compound in the same solution as in question 1 above that would have an absorbance of 1.5 in the same 1.00 cm cell is (in grams):

a. 0.050
b. $0.075 \log_{10} 2$
c. $0.033 \log_{10} 2$
d. $0.075 / \log_{10} 2$
e. $0.075 / \log_{10} 0.5$
f. none of the above

ANSWER:

According to Lambert-Beer law absorbances for two different situations can be expressed as:

$$A_1 = -\log\frac{I_1}{I_0} = \varepsilon_{\lambda 1} c_1 l_1 = \varepsilon_{\lambda 1} l_1 \frac{m_1}{V}$$

$$A_2 = -\log\frac{I_2}{I_0} = \varepsilon_{\lambda 2} c_2 l_2 = \varepsilon_{\lambda 2} l_2 \frac{m_2}{V}$$

where $\varepsilon_{\lambda 1} = \varepsilon_{\lambda 2} = \varepsilon_{\lambda}$, $l_1 = l_2 = 1\text{cm}$,
$A_1 = 1.5$ and $A_2 = -\log 0.5 = \log 2$

$$\frac{A_1}{A_2} = \frac{m_1}{m_2} \Rightarrow \frac{1.5}{\log 2} = \frac{m_1}{0.050g}$$

$$m_1 = 0.075 / \log 2 g$$

Question 3:

Indicate those of the following statements that are correct for the spectra of Prob #1:

1.The IR spectrum is consistent with the presence of a C=C group in the molecule.
False. There is no C=C group vibration in IR spectrum.
2.The mass spectrum peak at mass 83 is consistent with the loss of a methyl group fragment.
True. Since 98-83=15,which correspond to a methyl fragment.
3.The lack of a UV or visible spectrum is consistent with the molecule being a saturated dihalogenated hydrocarbon.
True. Saturated hydrocarbons do not show UV or VIS spectra.
4.The carbon-13 spectrum indicates that all carbons in the compound are equivalent, and that all carbons are directly attached to two protons.
False. There are two types of carbons in an molecule : CH one and CH_3 one according to a proton coupled 13C NMR spectra.
5.The proton NMR indicates that a group representing three protons is next to a group containing a single proton.
True. According to a splitting pattern there are two types of protons: CH and CH_3.
6.The proton NMR indicates that a group representing three protons is next to a group containing two protons.
False. According to a splitting pattern there are two types of protons: CH and CH_3.
7.The compound is CH_2XCH_2X where X is Cl or Br.
False.
8.The compound is CH_3CHX_2 where X is Cl or Br.
True.

Question 4:

Indicate those of the following statements that are correct for the spectra of Prob #2:

1.The IR is consistent with the presence of a C=C group in the molecule.
False. There is no C=C group vibration in IR spectrum.
2.The mass spectrum peak at mass 107 is consistent with the loss of a methyl group fragment.
False. Peak at mass 107 is a parent peak.
3.The lack of a UV or visible spectrum is consistent with the molecule being a saturated dihalogenated hydrocarbon.
True. Saturated hydrocarbons do not show UV or VIS spectra.
4.The carbon-13 NMR spectrum indicates that all carbons in the compound are equivalent, and that all carbons are directly attached to two protons.
True. There is only one peak in carbon-13 spectra indicating that all carbons are equivalent and splitting pattern is indicating that carbon is attached to two protons.
5.The proton NMR spectrum indicates that a group representing three protons is next to a group containing a single proton.
False. There is only one type of proton .
6.The proton NMR indicates that a group representing one proton is next to a group containing two protons.
False. There is only one type of proton .
7.The compound is CH_2XCH_2X where X is Cl or Br.
True.
8.The compound is CH_3CHX_2 where X is Cl or Br.
False.

Question 5:

Indicate those of the following statements that are correct for the compound $^{13}CH_3OH$:

1.The carbon-13 will be a 1:2:1 triplet.
False. Splitting pattern of carbon attached to three protons wolud give a 1:3:3:1 quartet.
2.The proton NMR spectrum will be a 1:1 doublet and a broad singlet.
True. Proton NMR would be a doublet for CH_3 due to 13C-H coulpling and a broad singlet for OH due to an exchange process.
3.The broad singlet in the proton spectrum is due to the exchange of protons among methanol molecules.
True.
4.Because of the oxygen, IR spectrum will have a strong band around 1750 cm^{-1}.
False. For molecules that contain the oxygen the possible regions in IR spectrum that indicate that are: first between 1630-1850 cm^{-1} for C=O strong stretch and second between 3590-3650 cm^{-1} that correspond to strong OH stretch. So presence of oxygen doesn't necessarily mean presence of 1750 cm^{-1} strong band that correspond to C=O.
5.This compound will absorb in the visible region, and will therefore be coloured.
False. The alcohol do not give an UV or VIS absorption.
6.The mass spectrum should have a peak at mass 15.
False. The possible peaks in mass spectra of carbon-13 methanol would be: a parent peak at 33 m/e, a peak at 17 m/e due to a loss of OH and at 16 m/e due to a loss of $^{13}CH_3$.