Organic Chemistry: Tutorial 3

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Part Four

Question #8

Spectrum 1

(a)

$0.50 : 0.50 : 0.50 : 0.95 : 1.50 \approx 1 : 1 : 1 : 2 : 3$

As there are a total of 8 Hydrogen in the compound, the probably number or protond corresonding to each peak is:

$1H, 1H, 1H, 2H, 3H$ (from least to most shielded)

(b)

1. $\delta = 6.42 - 6.38 : \underline{H_2}C = C$, doublet, $J = 3.50 \cdot 10^{-2}\delta$
2. $\delta = 6.15 - 6.09 : \overline{H_2}C = C\underline{H} -$ doublet of doublets, $J_1 = 4.0 \cdot 10^{-2}\delta, J_2 = 2.0 \cdot 10^{-2}\delta$
3. $\delta = 5.83 - 5.80 : \underline{H_2}C = C$ (cis to other H group) doublet,$J_1 = 2.0 \cdot 10^{-2}\delta, J_2 = 1.0 \cdot 10^{-2}\delta$
4. $\delta = 4.24 - 4.20 : \overline{O} - C\underline{H_2} - CH_3$ quartet,$J = 1.0 \cdot 10^{-2}\delta$
5. $\delta = 1.32 - 1.29 : -C\underline{H_3}$ triplet,$J = 1.5 \cdot 10^{-2}\delta$

Spectrum 2

(a)

$0.35 : 0.7 : 0.75 : 1.0 : 1.05 \approx 1 : 2 : 2 : 3 : 3$

As there are a total of 11 Hydrogens in the molecules the probably number of protins corresponding to each peak is:

$1H, 2H, 2H, 3H, 3H$ (from least to most shielded)

(b)

1. $\delta = 7.73 : \underline{H} - N$, singlet,
2. $\delta = 7.37 - 7.36 : Ar - C\underline{H}$ (by the N side of the ring) doublet, $J = 1.0 \cdot 10^{-2}$
3. $\delta = 6.82 - 6.80 : AR - C\underline{H}$ (by the O side of the ring) doublet, $J = 2.0 \cdot 10^{-2}$
4. $\delta = 4.01 - 3.96 : CH_3 - C\underline{H_2} - O$ quartet,$J = 1.5 \cdot 10^{-2}\delta$
5. $\delta = 2.11 : CO_2 - C\underline{H_3}$ singlet,
6. $\delta = 1.40 - 1.37 : C\overline{H}\underline{H_3} - CH_2$ triplet,$J = 2.5 \cdot 10^{-2}\delta$

Question #9

$CH_3 - CH_2 - CH_2 - CH_2 - OH$

$(CH_3)_3COH$

$(CH_3)_2CH - CH_2 - OH$

$CH_3 - CH(OH) - CH_2 - CH_3$

Isomer #1

$CH_3 - CH_2 - CH_2 - CH_2 - OH$

1. $\delta = 4.20 - 4.18 : \underline{H} - O$ triplet, 1H
2. $\delta = 3.61 - 3.57 : C\underline{H_2} - OH$ triplet, 2H
3. $\delta = 1.59 - 1.55 : CH_2 - C\underline{H_2} - CH_2$ pentuplet,2H
4. $\delta = 1.42 - 1.38 : CH_3 - C\underline{H_2} - CH_2$ sestuplet, 2H
5. $\delta = .98 - 0.89 : C\underline{H_3} - CH_2$ triplet, 1H

Isomer #2

$(CH_3)_3COH$

1. $\delta = 2.4518 : \underline{H} - O$ singlet, 1H
2. $\delta = 1.25 : (C\underline{H_3})_3C - OH$ singlet, 9H

Isomer #3

$(CH_3)_2CH - CH_2 - OH$

1. $\delta = 3.53 - 3.48 : \underline{H} - O$ triplet, 1H
2. $\delta = 3.40 - 3.33 : C\underline{H_2} - OH$ triplet, 2H
3. $\delta = 1.81 - 1.69 : (CH_3)_2C\underline{H} - CH_2-$ nonuplet,1H
4. $\delta = 0.93 - 0.87 : (C\underline{H_3})_2 - CH$ doublet, 6H

Question #10

1. $CH_3 - CH_2 - CH_2 - CH_2 - Cl$
2. $CH_3 - CH_2 - CH(Cl) - CH_3$
3. $(CH_3)_2 - CH - CH_2 - Cl$
4. $(CH_3)_3 = C(Cl)$

The first specta could correspond to either $CH_3-CH_2-CH_2-CH_2-Cl$, or $CH_3-CH_2-CH(Cl)-CH_3$ as it both contain the four unique signal seen in the same ranges. The second (right) spectra can only correspond to $(CH_3)_3 = C(Cl)$ as this is the only isomer in which there are only 2 unique carbon environments.

Part Five

Question #2

1. 87: $CH_2CO_2CH_3$
2. 71: CH_3CH_2CO

3. 59: CO_2CH_3
4. 43 $COCH_3$

Question #3

(i)

Molecular ion $m/z = 72$

Principle Fragments

1. 57: $CH_3CH_2CH_2CH_2$
2. 43 $CH_3CH_2CH_2$
3. 42 $CH_2CH_2CH_2$
4. 29 CH_3CH_2
5. 28 CH_2CH_2
6. 15 CH_3
7. 14 CH_2

P$(M+1)^+$ peak $=5C1 \cdot 0.011^1 \cdot 0.989^4 = 0.0526$

$0.0526 \cdot 40\% = 2.1\%$