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NMR Spectroscopy Problem

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Q-1) The molecular formula of the compound is C_3H_6O with NMR data as shown below

a) Siglet at 9.77 c (1H), J =2Hz

b) quartet at 2.5 c (2H), J =6Hz

c) Triplet at 1.2 c (3H), J =6Hz

Ans:- Sites of Unsaturation

$C_nH_{2n+2} = C_3H_{2x3+2} = C_3H_8$

$C_3H_8 - C_3H_6 = H_2$

therefore from the formula it is clear that there are 2H atoms less than the saturated hydrocarbon 2H/2=1 , hence there is one site of unsaturation.

a) The NMR signal at 9.77 corresponding to 1H atom indicates the presence of CHO group

b) The NMR signal at 2.5 corresponding to 2H atom indicates the presence of CH_2 group attached to CO group and CH_3 group therefore their signal at 2.5 splits into quarted

c) The NMR signal at 1.2 corresponding to 3H atom indicates the presence of CH_3 group attached to CH_2 group therefore their signal at 1.2 splits into triplet. The value of coupling constant J for data b and c are same . So the two carbon atom must be adjacent to each other.

Thus , the possible structure of the compound is propanaldehyde

CH_3-CH_2-CHO

Q-2) The molecular formula of the compound is C_3H_7NO with NMR data as shown below

a) c' 1.18 (s, 1H) b) c' 2.7 (s, 3H), c) c' 1.9 (s, 3H),

Ans:- Sites of Unsaturation

$C_nH_{2n+2} = C_3H_{2x3+2} = C_3H_8$

$C_3H_7\text{-}_1 = C_3H_6$

$C_3H_8\text{-}C_3H_6 = H_2$

therefore from the formula it is clear that there are 2H atoms less than the saturated hydrocarbon 2H/2=1 , hence there is one site of unsaturation.

a) The NMR signal at 1.18 corresponding to 1H atom indicates the presence of CH or NH group therefore their signal at 1.18splits into singlet

b) The NMR signal at 2.7 corresponding to 3H atom indicates the presence of CH_2 group attached to CO group therefore their signal at 2.7splits into singlet

c) The NMR signal at 1.9 corresponding to 3H atom indicates the presence of CH_3 group attached to N atom therefore their signal at 1.9 splits into singlet .

Thus , the possible structure of the compound is N-Methyl acetamide

$CH_3\text{-}CO\text{-}NH\text{-}CH_3$

Q-3) The molecular formula of the compound is C_7H_8 with NMR data as shown below

a) Siglet at 2.32 c° (3H)

b) Siglet at 7.17 c° (5H)

Ans:- Sites of Unsaturation

$C_nH_{2n+2} = C_7H_{2x7+2} = C_7H_{16}$

$C_7H_{16}-C_7H_8 = H_8$

therefore from the formula it is clear that there are 8H atoms less than the saturated hydrocarbon 8H/2=4 , hence there is four site of unsaturation.

a) The NMR signal at 2.32 corresponding to 3H atom indicates the presence of CH_3 group attached to phenyl ring therefore their signal at 2.32 splits into singlet.

b) The NMR signal at 7.17 corresponding to 5H atom indicates the presence of aromatic proton attached to CH_3 group therefore their signal at 7.17 splits into singlet.

Thus , the possible structure of the compound is toulene

$C_6H_5-CH_3$

Q-4) The molecular formula of the compound is $C_7H_7NO_2$with NMR data as shown below

a) 7.98 c (2H, doublet) b) 7.25 c (2H, doublet)) c) 2.40 c (3H, singlet)

Ans:- Sites of Unsaturation

$C_nH_{2n+2} = C_7H_{2x7+2} = C_7H_{16}$

$C_7H_{7-1} = C_7H_6$

$C_7H_{16}-C_7H_6 = H_{10}$

therefore from the formula it is clear that there are 10H atoms less than the saturated hydrocarbon 10/2=5 , hence there is five site of unsaturation.

a) The NMR signal at 7.98corresponding to 2H atom indicates the presence of aromatic proton attached to 1H therefore their signal at 7.98 splits into doublet.

b) The NMR signal at 7.25 corresponding to 2H atom indicates the presence of aromatic proton attached to 1H therefore their signal at 7.25 splits into doublet.

c) The NMR signal at 2.40 corresponding to 3H atom indicates the presence of CH_3 group attached to phenyl ring or CO group therefore their signal at 2.40 splits into singlet.

Thus , the possible structure of the compound is 4-Nitrotoulene

$NO_2-C_6H_4-CH_3$

Q-5) The molecular formula of the compound is $C_4H_7BrO_2$ with NMR data as shown below

a) 1.08 c (3H, t) b) 2.07 c (2H, m)) c) 4.2 c (1H, t) c) 10.97 c (1H, s)

Ans:- Sites of Unsaturation

$C_nH_{2n+2} = C_4H_{2x4+2} = C_4H_{10}$

$C_4H_{7+1} = C_4H_8$

$C_4H_{10} - C_4H_8 = H_2$

therefore from the formula it is clear that there are 2H atoms less than the saturated hydrocarbon 2/2=1 , hence there is one site of unsaturation.

a) The NMR signal at 1.08 corresponding to 3H atom indicates the presence of CH_3 attached to CH_2 group therefore their signal at 1.08 splits into triplet.

b) The NMR signal at 2.07 corresponding to 2H atom indicates the presence of multiple proton attached therefore their signal at 2.07 splits into multiplet.

c) The NMR signal at 4.2 corresponding to 1H atom indicates the presence of CH group attached to CH_2 group therefore their signal at 4.2 splits into triplet.

d) The NMR signal at 10.97 corresponding to 1H atom indicates the presence of acid proton group therefore their signal at 10.97 splits into singlet.

Thus , the possible structure of the compound is 2-bromobutanoic acid

CH_3-CH_2-CHBr-COOH