(3) Problems pertaining to the structure elucidation of simple organic compounds using PMR spectroscopic data (Supporting IR & UV data to be given)

(a) M.F C_3H_8O

UV - 174 nm (ϵ_{max} - 10,000)

IR : 1050 cm^{-1}, 2850, 2970 & 3400 cm^{-1}.

^{1}H-NMR :

δ 1.0 (3H, t)

δ 1.2 (2H, sextet)

δ 3.2 (2H, t)

δ 5.0 (1H, s. exchengeble with D_2O)

Soln :

M.F C_3H_8O

$DBE = n+1 - Y/2 = 3+1 - 8/2 = 4-4$

$= 0$

UV - 174 nm (ϵ_{max}-10,000) - It shows the $\pi \rightarrow \pi^*$ trasitions.

IR

1050 cm^{-1} :. It shows the C-O stretching band of primary alcohol.

2850 & 2970 cm^{-1} - It shows the C-H Symmetric & asymmetric stretching bands of $-CH_3$ group.

3400 cm^{-1} - It shows the -O-H stretching band of alcohol.

^1H - NMR.

δ 1.0 (3H, t) — It indicate CH_3-CH_2 group

δ 1.2 (2H, sextet) - It indicate $CH_3-CH_2-CH_2$

δ 3.2 (2H, t,) - It indicate $CH_3-CH_2-CH_2-O$

δ 5.0 (1H, s, exchengeblewith D_2O) · CH_2-OH

The above spectral data the structure of the compound is.

$CH_3-CH_2-CH_2-OH$

1- propanol.

(b) M.F. C_3H_8O

UV - 174 nm.

IR, : 1100, 2850, 2970 & 3400 cm^{-1}.

^1H - NMR : (δ in ppm)

1. δ 1.2 (6H, d)

2. δ 3.2 (1H m)

3. δ 5.0 (1H, s)

-soln M.F. C_3H_8O

DBE = $4 - 8/2 = 4-4 = 0$

UV - 174 nm - It shows the $n \rightarrow \sigma^*$ transition

IR : 1100 cm^{-1}. - It indicate C-O stretching b of secondary alcohols.

2850 & 2970 cm^{-1}. It show C-H symmetric & asymmetric stretching of

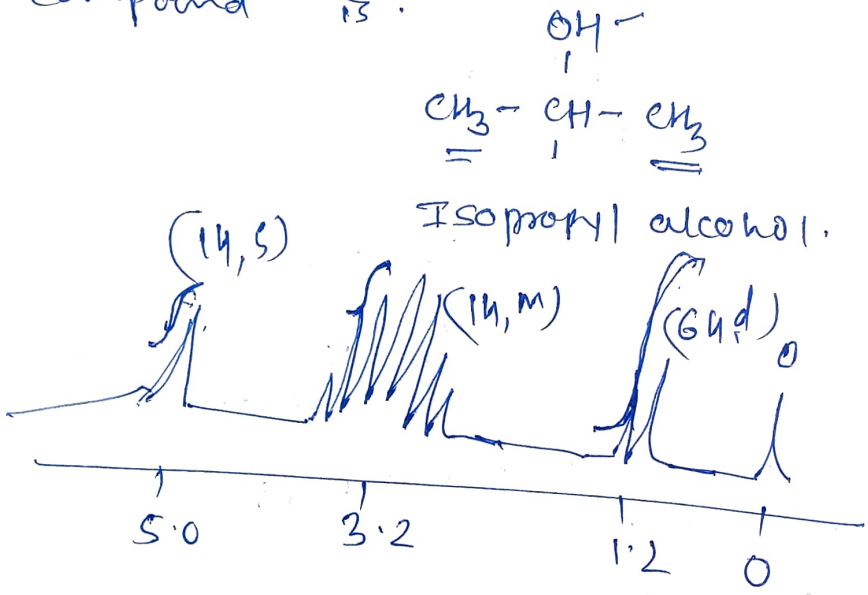
^1H- NMR :

δ 1.2 (d, 6H) - It shows the $\frac{CH_3}{CH_3}$>CH - group

δ 3.2 (m, 1H) $CH_3-\underline{CH}-CH_3$ group.

δ 5.0 (1H, S) It shows the -OH.

The above spectral data the structure of the compound is.



(c) M.F. $C_4H_{10}O$

UV - 180 nm

IR, 1150, 3400 & 2850, & 2970 cm^{-1}.

^1H-NMR:

δ 1.5 (S, 9H)

δ 5.2 (S, 1H)

Soln :

M.F. $C_4H_{10}O$

$DBE = n+1-Y/2 = 4+1-10/2 = 5-5 = 0$

UV - 180 nm - It shows the $n \rightarrow \sigma^*$ transition is present

IR 1) 1150 cm^{-1} - C-O stretching band of tertiary alcohol

2) 3400 cm^{-1} - It shows the O-H stretching of alcohol

3. 2850 & 2970 cm^{-1}. – It shows the C–H symmetric & asymmetric stretch of $-CH_3$ group.

^1H-NMR. (δ in ppm)

δ 1.5 (S, 9H) It indicate the $CH_3-\overset{CH_3}{\underset{|}{C}}-CH_3$

δ 5.2 (S, 1H) It indicate the $-OH$

The above spectral data shows the structure of compound is

$CH_3-\overset{CH_3}{\underset{CH_3}{C}}-OH$ tertiary butyl alcohol.

(d) Deduce the structure, if given following spectral data.

M.F. $C_2H_4O_2$

UV – 210 nm ($\epsilon_{max.}$ - 50)

IR :- 1720, 3000 – 2500 cm^{-1}, & 1200 cm^{-1}.

^1H-NMR - δ 2.5 (S, 3H)

δ 10.5 (S, 1H, exchangeable with D_2O)

Soln :-

M.F $C_2H_4O_2$

DBE $= 2+1-4/2 = 3-2 = 1$,

UV : 210 nm (ϵ_{max} - 50) – It shows the $n \rightarrow \pi^*$ transition.

IR :- 1. 1720 cm^{-1} – C=O stretching band of acids.

2. 3000 – 2500 cm^{-1} – It shows O–H stretching band of acid

3. 1200 cm^{-1} – It shows the C–O stretch band of acid.

^{1}H-NMR

δ 2.5 (S, 3H) — adjacent $-\overset{O}{\overset{\|}{C}}-CH_3$

δ 10.5 (S, 1H, exchangeable with D_2O) — $-COOH$

The structure is.

$$CH_3-\overset{O}{\overset{\|}{C}}-OH$$

(e) M.F. C_2H_7N.

UV — 190 nm

IR — 1400 cm^{-1}, 3300 & 3400 cm^{-1}.

^{1}H-NMR: (δ in ppm)

δ 1.2 (3H, t)

δ 3.0 (2H, q)

δ 4.0 (2H, S, exchangeable with D_2O)

Soln M.F. C_2H_7N

$$DBE = 2+1-\frac{Y-No.of\ N\text{-}atom.}{2}$$

$$= 2+1-\frac{7-1}{2} = 3-3 = 0$$

1, UV — 190 nm. shows the $n \rightarrow \sigma^*$ transitions.

2. IR - 1. 1400 cm^{-1} : It shows the C-N stretching bands of amine

2. 3300 & 3400 cm^{-1} : It shows the N-H symmetric & asymmetric stretching of $-NH_2$ group.

^{1}H-NMR

δ 1.2 (t, 3H) — CH_3-CH_2

δ 3.0 (q, 2H) — CH_2-CH_3

δ 4.0 (S, 2H, exch. D_2O) — NH_2

The structure of the comp. is.

$CH_3 - CH_2 - NH_2$

Ethyl amine.

(f) M.f. C_3H_5N.

UV - 230 nm (ϵ_{max} - 60)

IR - 2250 cm^{-1}, 2860 & 2970 cm^{-1}.

^1H-NMR :- δ 1.2 (3H, t)

3.2 (2H, q)

Soln M.f. = C_3H_5N.

$$DBE = x + 1 - \frac{y - NO.\text{ of } N.\text{atom}}{2}$$

$$= 3 + 1 - \frac{5-1}{2} = 4 - 4/2 = 4 - 2$$

DBE = 2

UV - 230 nm (ϵ_{max} 60) → It shows the $n \rightarrow \pi^*$

IR - 2250 cm^{-1} - It shows the C≡N stretch cyanide.

2860 & 2970 cm^{-1} - It shows the C-H symmetric & asymmetric stretching of CH_3 group.

^1H-NMR - δ 1.2 (3H, t) = It shows the CH_3-CH_2

δ 3.2 (2H, q) It shows the CH_2-CH_3

structure

$CH_3 - CH_2 - C \equiv N$

(9) M.F. C_4H_8O

UV – 283 nm (ϵ_{max} – 20)

IR – 1715 cm^{-1}, 2970 & 2860 cm^{-1}

PMR – (δ, ppm)

δ 1.3 (t, 3H, J = 7Hz)

δ 2.4 (q, 2H, J = 7Hz)

δ 2.3 (s, 3H).

Soln

M.F. = C_4H_8O

$DBE = 2+1-H/2 = 4+1-8/2 = 5-4 = 1$

UV – 283 nm (ϵ_{max} – 20) – It shows the $n \rightarrow \pi^*$ transitions.

IR

1715 cm^{-1} – It indicate the C=O stretching of band of ketones.

2970 & 2860 cm^{-1} – It shows the C–H asymmetric & symmetric stretching bands of alkyl group.

PMR (δ ppm)

δ 1.3 (t, 3H, J = 7Hz) It shows CH_3-CH_2

δ 2.4 (q, 2H, J = 7Hz) It shows CH_2-CH_3

δ 2.3 (s, 3H) It shows $C(=O)-CH_3$

The above spectral data the structure of the comp. is.

$CH_3-CH_2-C(=O)-CH_3$.

(b) M.F. $C_4H_8O_2$

UV - 230 nm (ϵ_{max} 60)

IR. 1745, 1060 & 1200 cm^{-1}.

NMR:

δ 2.3 (s, 3H)

δ 3.5 (q, 2H)

δ 1.7 (t, 3H)

Soln M.F. $C_4H_8O_2$ DBE = 1

UV - 230 nm (ϵ_{max} 60) - It shows the $n \rightarrow \pi^*$ transitions.

IR:

1745 cm^{-1} - $\overset{O}{\overset{\|}{C}}$ stretching band & ester.

1060 & 1200 cm^{-1} - It shows the C-O stretching bonds & ester group.

NMR (δ PPM)

δ 2.3 (s, 3H) - It shows $CH_3-\overset{O}{\overset{\|}{C}}$

δ 3.5 (q, 2H) - It shows the $O-CH_2-CH_3$

δ 1.7 (t, 3H) - It indicates the CH_3-CH_2-O

The above conclusion the structure of the comp. is.

s O q t

$CH_3-\overset{O}{\overset{\|}{C}}-O-CH_2-CH_3$

(i) M.f. C_8H_{10}

UV - 200 nm (ϵ_{max} 10,000)

IR - 3030 cm^{-1}, 1600, 1550, 1400 cm^{-1}.

^1H-NMR (δ PPM):

δ 1.2 (3H, t)

δ 2.5 (2H q)

δ 7.2 (5H, s)

Soln M.f. C_8H_{10}

$DBE = 8 + 1 - 10/2 = 9 - 5 = 4$

UV - 200 nm (ϵ_{max} 10000) → It show the $\pi \rightarrow \pi^*$ trasition.

IR - 3030 cm^{-1} - Aromatic C-H stretching band.

1600, 1550 & 1400 cm^{-1} - It show the Aromatic C=C stretching bands.

^1H-NMR (δ PPM)

δ 1.2 (3H, t) — It shows the $\underline{CH_3}$-CH_2

δ 2.5 (2H q) — It shows the C-$\underline{CH_2}$-CH_3

δ 7.2 (5H, s) - It indicates 

The above conclusion structure of the comp. is

Ethyl benzene

(j) M.F C_8H_8O

UV - 275 nm (ϵ_{max} 20)

IR : 2720, 2820, 1720, 1600, 1499, 1450 cm^{-1}.

^1H-NMR. (δ ppm)

δ 2.4 (d, 2H)

δ 9.7 (t, 1H)

δ 7.2 - 7.9 (m, 5H)

Soln

M.f. - C_8H_8O

DBE = $x + 1 - y/2 = 8 + 1 - 8/2 = 9 - 4 = 5$

UV - 275 nm (ϵ_{max} 20) - It shows the $n \rightarrow \pi^*$ transition.

IR :

2720 & 2820 cm^{-1} - C-H stretching bands of aldehyde.

1720 - $\overset{O}{\overset{\|}{C}}$ - stretching of aldehydic group.

1600, 1499, & 1450 cm^{-1}. - Aromatic C=C stretching bands.

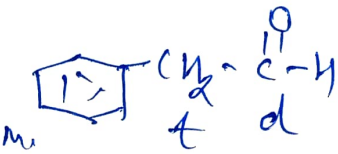
^1H-NMR data : (δ ppm)

δ 2.4 (d, 2H) - $C-\underline{CH_2}-\overset{O}{\overset{\|}{C}}-H$

δ 9.7 (t, 1H) - $C-CH_2-\overset{O}{\overset{\|}{C}}-H$

δ 7.2 - 7.9 (m, 5H) - 

The above spectral data structure of the comp. is,



M.f.

(K) C_6H_6O

UV - 220 nm (ϵ_{max} - 10,520)

IR - 1200 cm^{-1}, 1600, 1450, 1400, 3030, ~~1200~~, & 3395 cm^{-1}.

PMR (δ ppm) :

δ 8.0 (S, 1H)

δ 6.8 - 7.5 (m, 5H)

Soln :- M.F. C_6H_6O

DBE = $6+1-6/2 = 7-3 = 4$

UV - 220nm (ϵ_{max} 10,520) → $\pi \rightarrow \pi^*$ transition.

IR.

1200 cm^{-1}. - C-O stretching band of phenol

1600, 1450 & 1400 cm^{-1} - It shows the aromatic C=C stretching band.

3030 cm^{-1} Aromatic C-H stretching band.

3395 cm^{-1} - It show the O-H stretching band of phenol

PMR (δ ppm)

δ 8.0 (S, 1H) It shows the Ar-OH

δ 6.8 - 7.5 (m, 5H) It shows the 

The structure is.

Phenol.

(2) M.f. C_3H_8O

UV - 170 nm.

IR : 1050 cm^{-1}, 2960, & 2850 cm^{-1}.

PMR (δ ppm)

δ 1.2 (t 3H $J = 6.5\ Hz$)

δ 3.5 (q, 2H, $J = 6.5\ Hz$)

δ 3.0 (s, 3H).

Soln M.f. C_3H_8O

$DBE = x + 1 - y/2 = 3 + 1 - 8/2$

$= 4 - 4 = 0$

UV - 170 nm → $n \rightarrow \sigma^*$ transitions.

IR - 1050 cm^{-1} - C-O stretching band of ether

2960 & 2850 cm^{-1} - CH asymmetric & symmetric stretching bands of alkyl group.

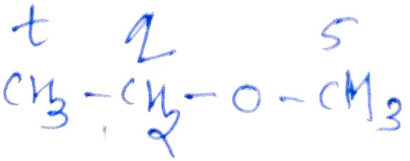
PMR (δ ppm)

δ 1.2 (t, 3H, $J = 6.5\ Hz$) $CH_3 - CH_2$

δ 3.5 (q, 2H $J = 6.5\ Hz$) $O - CH_2 - CH_3$

δ 3.0 (s, 3H) It shows the $-OCH_3$

The Structure of comp B



Ethyl methyl ether

(M) M.F. $C_2H_6O_2$

UV - 175 nm.

IR - 3400 cm^{-1}, 1050 cm^{-1}.

PMR (δ ppm)

δ 3.7 (4H, s)

δ 2.5 (2H, s)

Soln M.F. $C_2H_6O_2$

$DBE = 2+1-6/2 = 3-3 = 0$

UV - 175 nm → It shows $n \rightarrow \sigma^*$ trasition.

IR - 3400 cm^{-1}. O-H stretching band of alcohol.

1050 cm^{-1}. C-O stretching band of primary alcohol.

PMR (δ ppm)

δ 3.7 (4H, s) It shows $-CH_2-$

δ 2.5 (2H, s) It shows $-CH_2-$

OH OH

Structure is

$HO-CH_2-CH_2-OH$

(n) C_3H_7NO

UV - 230 nm (ϵ_{max} 60)

IR - 1680 cm^{-1} 1400 cm^{-1} + 3300, 3400 cm^{-1}.

PMR (δ ppm)

δ 1.7 (3H, t)

δ 2.5 (2H, q)

δ 5.5 (2H, s. exchangeable with D_2O)

Soln M.F. C_3H_7NO

$$DBE = x + 1 - \frac{y - No.\ of\ N\text{-}atom}{2}$$

$$= 3 + 1 - \frac{7-1}{2} = 4 - 6/2 = 4 - 3 = \underline{1}$$

UV - 230 nm (ϵ_{max} 60) → $n \rightarrow \pi^*$ transition

IR - 1680 cm^{-1} - C=O stretching band of amide

1400 cm^{-1} - C-N stretching band of amide

3300 & 3400 → N-H stretching bands of $-NH_2$ group of amide.

δ 1.7 (3H, t) It show the CH_3-CH_2-

δ 2.5 (2H, q) It show the $-\overset{O}{\overset{\|}{C}}-CH_2-CH_3$

δ 5.5 (2H, s exchegeble with D_2O) $-\overset{O}{\overset{\|}{C}}-NH_2$

The structure is

$$CH_3-CH_2-\overset{O}{\overset{\|}{C}}-NH_2$$

(c) M.F. C_3H_6O

UV - 295 nm (ϵ_{max} 60)

IR. 2720, 2820, 1720 cm^{-1}.

PMR (δ ppm)

δ 1.3 (t, 3H $J = 6.5$ Hz)

δ 2.4 (quin, 2H, $J = 6.5$ Hz)

δ 9.7 (t, 1H)

Soln: M.F. C_3H_6O

$$DBE = x + 1 - y/2$$
$$= 3 + 1 - 6/2 = 4 - 3 = 1$$

UV - 295 nm (ϵ_{max} 60) - It shows the $n \rightarrow \pi^*$ trasition.

IR - 2720 & 2820 cm^{-1} - It shows the C-H stretching bands of aldehyde group.

1720 cm^{-1} - $\overset{O}{\overset{\|}{C}}$- stretching band of aldehyde.

PMR (δ ppm):

δ 1.3 (t, 3H $J = 6.5$ H.) - It shows CH_3-CH_2

δ 2.4. (quin, 2H $J = 6.5$) $CH_3-CH_2-\overset{O}{\overset{\|}{C}}H$

δ 9.7 (t, 1H) It shows the $CH-CH_2$

The above conclusion the structure of the comp. is.

$$CH_3-CH_2-\overset{O}{\overset{\|}{C}}-H.$$
t quin t