Problem O, \( \text{C}_5\text{H}_{10}\text{O}_2 \)

\[
\text{DBE} = \frac{\left(\left(2 \times 5\right) + 2\right) - 10}{2} = 1
\]

2 'O' and IR peak at 1740 suggests: ester = 1DBE
Integration ratios: \[ 2 : 3 : 2 : 3 = 10 \]

δ 4 - what can shift a CH₂ down to 4? only –O–
$\text{C}_5\text{H}_{10}\text{O}_2$

but this is a triplet

so it is next to another CH$_2$

but this is a sextet
$C_5H_{10}O_2$

but this is a sextet
so it is next to $6-1 = 5$ H’s

only one peak left

$\text{a – CH}_3$!!
\[\text{C}_5\text{H}_{10}\text{O}_2\]

always check to see shifts are reasonable

1 1.3+0.5 3.5+0.5 2.3

could have started here

p. 123
Problem P  \( \text{C}_6\text{H}_{12}\text{O} \)

\[ \text{DBE} = \frac{\{(2\times6)+2\}-12}{2} = 1 \]

1 ‘O’ and IR peak at 1720 suggests: \( >\text{C}=\text{O} \)

what sort of carbonyl?  

NO 2750 peak, so probably ketone

how do we verify this – look in \( ^1\text{H} \) NMR for –CHO at \( \delta \) 10
Problem P   $\text{C}_6\text{H}_{12}\text{O}$

no $\delta$ 10, so must be a ketone.

Integrations: $2:3:2:2:3 = 12$

$\delta$ 1 = -CH$_3$ – a triplet so next to a –CH$_2$-, so we have a –CH$_2$CH$_3$

we now have to decide is this the triplet, quintet or the sextet, which are all –CH$_2$- ????
try different approach – only functional group is ketone

$\text{CH}_x\text{-CO-CH}_y$  H’s next to a ketone are in 2-3 region

so we have a $-\text{CH}_2-$ and a $-\text{CH}_3$

so we now know we have $\text{CH}_3\text{-CO-CH}_2$.
Problem P  \( \text{C}_6\text{H}_{12}\text{O} \)

Integrations: 2:3:2:2:3 = 12

\(-\text{CH}_2\text{CH}_3\) so we now know we have \(\text{CH}_3\text{-CO-CH}_2\)-

triplet, so next to \(-\text{CH}_2\)-

\(\text{CH}_3\text{-CO-CH}_2\text{-CH}_2\)- but don’t forget we have already found a \(-\text{CH}_2\text{-CH}_3\)

so now we have found all six carbons!!
Problem P  $\text{C}_6\text{H}_{12}\text{O}$

Integrations: $2:3:2:2:3 = 12$

CH$_3$-CO-CH$_2$-CH$_2$-CH$_2$-CH$_2$-CH$_3$ so they must be joined!

CH$_3$-CO-CH$_2$-CH$_2$-CH$_2$-CH$_2$-CH$_3$ now check splittings, and $\delta$

- $s$ 5 6 $t$ <= expect
- $\delta$ 2.3 2.5 1.3 0.9 <= expect

between 2 and 1.3
Problem Q  \( \text{C}_5\text{H}_{10}\text{O}_2 \)

\[
\text{DBE} = \frac{\left\{\left[(2 \times 5) + 2\right] - 10\right\}}{2} = 1
\]

2 ‘O’ and IR peak at 1740 suggests:  ester  = 1DBE
Problem Q  $\text{C}_5\text{H}_{10}\text{O}_2$

Integrations:  3 :  2 :  2 :  3  = 10H

Ester

Most downfield peak will be on –O- so

Next to a carbonyl is 2-3, so
Problem Q  \( \text{C}_5\text{H}_{10}\text{O}_2 \)

Integrations: 3 : 2 : 2 : 3 = 10H

\( \text{CH}_3\text{-O-} \text{C} - \text{CH}_2 \) <= triplet, so next to \(-\text{CH}_2\)-

\( \text{CH}_3\text{-O-} \text{C} - \text{CH}_2\text{-CH}_2 \) <= sextet, so next to 5H

2 + 3
Problem Q \( \text{C}_5\text{H}_{10}\text{O}_2 \)

Integrations: \( 3 : 2 : 2 : 3 = 10\text{H} \)

\[
\begin{align*}
\text{CH}_3 & \quad \text{O} \quad \text{C} \quad \text{CH}_2 & \quad \text{CH}_2 & \quad \text{CH}_3 \\
\text{singlet} & \quad \text{triplet} & \quad \text{triplet} & \quad \text{sextet}
\end{align*}
\]

check data
Problem R  $\text{C}_5\text{H}_{12}\text{O}$

$\text{DBE} = \frac{\{(2 \times 5) + 2\} - 12}{2} = 0$

1 'O' but no $-\text{OH}$ or $\text{C}=\text{O}$

so ether – there is an 1100 C-O str
Problem R  $C_5H_{12}O$  Integrations $2:3 : 2:2:3 = 12H$

ether = C-O-C  so most downfield H’s next to O

$CH_3$-O  = singlet  $CH_2$ is triplet so next to $CH_2$

so $CH_3OCH_2CH_2^-$  most likely this is the next peak

but to be sure, we can now go to the end
Problem R  $\text{C}_5\text{H}_{12}\text{O}$  Integrations $2:3 : 2:2:3 = 12\text{H}$  

so $\text{CH}_3\text{OCH}_2\text{CH}_2-$  

$\text{CH}_3$ triplet so next to $-\text{CH}_2-$  

= $-\text{CH}_2\text{CH}_3$  

but we have now found all 5 carbon atoms 

so $\text{CH}_3\text{OCH}_2\text{CH}_2-\text{CH}_2\text{CH}_3$  

s  t  5  6  t $<=$check !!!
**Problem S  C₈H₉BrO**

DBE = \( \frac{[(2 \times 8) + 2] - (9 + 1)}{2} = 4 \)  > 6C, \( \delta \) 7 so benzene para (maybe)

functional group = -OH
Problem S  $\text{C}_8\text{H}_9\text{BrO}$

Integrations: $2:2 : 1 : 1 : 3 = 9$

- $\text{-OH, -Br, benzene (para, maybe)}$

para-benzene = $\text{C}_6\text{H}_4$
so $\text{C}_8\text{H}_8-\text{C}_6\text{H}_4$ left to find
= $\text{C}_2\text{H}_4$

OH do not couple

confirmed
Problem S  C$_8$H$_9$BrO

Integrations: 2:2 : 1 : 1 : 3 = 9

-\text{OH}, -\text{Br},

\text{para-benzene} = C_6H_4
\text{so } C_8H_8-C_6H_4 \text{ left to find } = C_2H_4

we have a CH (q next to 3) and a CH$_3$ (d next to 1)

so $\text{\textgreater CHCH}_3$
Problem $\text{S} \quad \text{C}_8\text{H}_9\text{BrO}$

Integrations: $2:2 : 1 : 1 : 3 = 9$

-OH, -Br,  \[ \begin{array}{c}
X \\
\text{Y}
\end{array} \] -CHCH$_3$
Problem S  \( \text{C}_8\text{H}_9\text{BrO} \)

\[
\begin{align*}
\text{Br} & \quad \text{OH} \\
\text{H} & \quad \text{CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{HO} & \quad \text{Br} \\
\text{H} & \quad \text{CH}_3
\end{align*}
\]

normal  \( \delta \sim 7.3 \)

shielded  \( \delta 6.8 \)

as well, Ar-OH  \( \delta 5-10 \)
and Ar-OH has IR 1220
not at around 1100

p. 127
Problem T \hspace{5mm} C_{11}H_{12}

\[ DBE = \frac{[(2 \times 11) + 2] - (12)}{2} = 6 \]

\[ \delta 7 \] so benzene

two bands, so MONO

\[ 2200 = ? \]

\[ \text{C--C=\equiv C--C} \]

\[ = 6 \text{ DBE} \]
Problem \( T \quad \text{C}_{11}\text{H}_{12} \)

Integrations 5 : 2 : 2 : 3 = 12

these are all coupled so not

\[ \text{singlet} \]

p. 128
Problem T  $C_{11}H_{12}$

Integrations 5 : 2 : 2 : 3 = 12

these are all coupled so not

$C_3$

singlet
Integrations 5 : 2 : 2 : 3 = 12

CH$_3$ is a triplet, so is next to a CH$_2$, which is a sextet so must have 5 neighbors, 3 of which are CH$_3$, so other 2 must be –CH$_2$
Problem T \( \text{C}_{11}\text{H}_{12} \)

Integrations \( 5 : 2 : 2 : 3 = 12 \)

\[
\text{Integrations } 5 : 2 : 2 : 3 = 12
\]
Problem U  $\text{C}_8\text{H}_{10}\text{ClN}$

$$\text{DBE} = \frac{[(2 \times 8)+2+1]-(10+1)}{2} = 4 \quad > 6 \text{ C, } \delta \text{ 7 so benzene}$$

so use NMR

Functional group

$\text{-NH}_2$
Note the ‘leaning’ shape

Integrations: 2:2

-Cl, -NH₂

should be singlet, no coupling

para-benzene = C₆H₄

we still need to find C₈H₁₀ClN – C₆H₆ClN = C₂H₄

-CH₂-CH₂-
Problem U  C₈H₁₀ClN

Integrations: 2:2  2:2  2  = 10

-Cl, -NH₂

always then join bifunctional or higher groups together
Problem U  \( \text{C}_8\text{H}_{10}\text{ClN} \)

Integrations: 2:2

-Cl, -NH\(_2\), \( \text{CH}_2\text{CH}_2 \)

now, 2 choices

\( \text{Cl} \)-\( \text{CH}_2\text{CH}_2\)-\( \text{NH}_2 \)

\( \text{NH}_2 \)-\( \text{CH}_2\text{CH}_2\)-Cl

p. 129
Problem U  C₈H₁₀ClN

Integrations: 2:2  2:2  2 = 10

δ 7-7.3

correct

at least δ 3.5

shielded to 6.8

NH₂ ─── CH₂CH₂ ─── Cl

δ 7-7.3
Problem V  $C_9H_9N$

DBE = $\frac{[(2\times9)+2+1]-(9)}{2} = 6 > 6C$, $\delta 7$ so benzene maybe mono?

Functional Group?

-\textbf{CN}  Nitrile and benzene account for all DBE
Problem V  $\text{C}_9\text{H}_9\text{N}$

Integrations: $5 : 1 : 3 = 9$

mono-subs-benzene

$\text{C}_9\text{H}_9\text{N} - (\text{C}_6\text{H}_5 + \text{CN}) = \text{C}_2\text{H}_4$

so $>\text{CHCH}_3$

$q, d$
Problem V  $C_9H_9N$

Integrations: 5  :  1  :  3  = 9

$\text{phenyl} - >CHCH_3$

$\text{phenyl} - C≡N$

$\text{phenyl} - CH_3 - C≡N - H$
Problem W  \( \text{C}_{10}\text{H}_{12}\text{O} \)

DBE = \( \frac{[2\times10]+2-12]}{2} = 5 \)

>6 C, \( \delta \) 7 so benzene probably mono-subs

Functional Group?

ketone – confirm in NMR with no \( \delta \) 10

What sort of ketone?  >1700, satd, so?
Problem W  \( \text{C}_{10}\text{H}_{12}\text{O} \)

Integrations:  5  :  2  :  2  :  3  =  12

satd ketone, not next to benzene ring

CH\(_3\) triplet so next to CH\(_2\) –which?
Problem W  \( \text{C}_{10}\text{H}_{12}\text{O} \)

**Integrations:**  \( 5 : 2 : 2 : 3 = 12 \)

- **C\text{6}**
- **C\text{3}**
- \( -\text{CH}_2\text{CH}_3 \)
- next to anything else?
- **CC = C\text{11} !!!**

\( \delta = 2-3, \text{ so on carbonyl} \)
Problem W  \( \text{C}_{10}\text{H}_{12}\text{O} \)

Integrations:  \( 5 : 2 : 2 : 3 = 12 \)

\[
\begin{align*}
\text{multiplets} & \\
\text{singlet} & \\
\text{triplet} & \\
\text{quartet} & \\
\end{align*}
\]

\[
\begin{align*}
\text{O} & \\
\text{C} & \text{C} & \text{CH}_2 & \text{CH}_3 & \\
\text{δ} & 2.5 & 1
\end{align*}
\]
Problem X  \( \text{C}_9\text{H}_{10}\text{O} \)

\[
\text{DBE} = \frac{\{(2 \times 9) + 2\} - 10}{2} = 5 > 6 \text{ C}, \ \delta 7 \text{ so benzene}
\]

Functional group ? >C=O 2750, so –CHO confirm in NMR
Problem X  \( \text{C}_9\text{H}_{10}\text{O} \)

\[ \frac{1}{2} : \frac{2}{2} \]

\( \delta \) 10 confirms CHO

confirms para-benzene ring \( \text{C}_6\text{H}_4 \)

Have found \( \text{C}_7\text{H}_5\text{O} \), so \( \text{C}_2\text{H}_5 \) left to find

\(-\text{CH}_2\text{-CH}_3\)

\( q \)  \( t \)

\[ 2 : 3 = 10 \]
Problem X  \( \text{C}_9\text{H}_{10}\text{O} \)

\[
\begin{align*}
1 & : 2 : 2 \\
\text{OHC-} & \quad \text{-CH}_2\text{-CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{CH}_3 & -\text{CH}_2 \\
& \quad \text{CHO} \\
\end{align*}
\]

\( \delta 7.8 \)
Problem Y  $\text{C}_{10}\text{H}_{12}\text{O}_{2}$  

DBE = \frac{[(2 \times 10) + 2] - 12}{2} = 5  

> 6 C, δ 7 so benzene mono subst

Functional group = ester

can we tell what type of ester???

1740, so saturated both sides!!!
Problem Y \( \text{C}_{10}\text{H}_{12}\text{O}_{2} \)

Integrations 5 : 3 : 2 : 2 = 12H

\( \text{C}_7\text{H}_5\text{O}_2 \) so \( \text{C}_3\text{H}_7 \) left to find

\( \delta \) 3.5 so on O

\text{coupled}
Problem Y  C_{10}H_{12}O_2

Integrations  5  :  3  :  2:2  = 12H

CH_3-O-C  \quad \text{CH}_2\text{CH}_2  \quad \text{phenyl}

CH_3-O-C-\text{CH}_2\text{CH}_2-\text{phenyl}
DBE = \frac{\{(2 \times 11) + 2\} - 14}{2} = 5

> 6 \text{ C, } \delta 7 \text{ so benzene ?-subst}

Functional group = acid

type of acid??? <1700, so conjugated (to what)

benzene ring
Problem Z \[ C_{11}H_{14}O_2 \]

Integrations 2:2 : 9 = 13

-COOH is at $\delta$ 10-16 not shown in above spectrum

Benzene is para

\[ \text{C}_7\text{H}_5\text{O}_2 \quad \text{C}_4\text{H}_9 \]
Problem Z  \( \text{C}_{11}\text{H}_{14}\text{O}_{2} \)

Integrations 2:2

\[ 9 = 13 \]

\( (\text{CH}_3)_3 \) identical

\( -\text{C}(\text{CH}_3)_3 \)

\( 9H \sim \delta 1 \)