1.

(a) 

\[
\begin{align*}
\text{butan-2-one} & \quad \text{Low resolution MS: molar mass } = \text{72 g mol}^{-1} \\
&(\text{C}_4\text{H}_8\text{O}) \\
\text{IR: } \sim1700 \text{ cm}^{-1} \text{ for C}=\text{O}
\end{align*}
\]

\[
\begin{align*}
\text{butan-2-ol} & \quad \text{Low resolution MS: molar mass } = \text{74 g mol}^{-1} \\
&(\text{C}_4\text{H}_{10}\text{O}) \\
\text{IR: } \sim3300 \text{ cm}^{-1} \text{ (broad) O-H}
\end{align*}
\]

(b) 

\[
\begin{align*}
\text{(E)-penta-1,3-diene} & \quad \text{UV: conjugated double bonds leads to strong absorption}
\end{align*}
\]

\[
\begin{align*}
\text{penta-1,4-diene} & \quad \text{UV: double bonds are not conjugated so no strong absorption}
\end{align*}
\]

(c) 

\[
\begin{align*}
\text{cyclopentane} & \quad \text{Low resolution MS: molar mass } = \text{70 g mol}^{-1} \\
&(\text{C}_5\text{H}_{10})
\end{align*}
\]

\[
\begin{align*}
\text{pentane} & \quad \text{Low resolution MS: molar mass } = \text{72 g mol}^{-1} \\
&(\text{C}_5\text{H}_{12})
\end{align*}
\]

(d) 

\[
\begin{align*}
\text{acetic acid} & \quad \text{IR: } \sim3300 \text{ cm}^{-1} \text{ (very broad) O-H, } \sim1700 \text{ cm}^{-1} \\
& \text{C}=\text{O}
\end{align*}
\]

\[
\begin{align*}
\text{methyl formate} & \quad \text{IR: } \sim1700 \text{ cm}^{-1} \text{ C}=\text{O}
\end{align*}
\]

\(^1\text{H}\) and \(^{13}\text{C}\) NMR could be used in all cases.
2. (a) A, B and C would all give three signals in the $^1H$ NMR spectrum
(b) E possesses a $^1H$ NMR spectrum consisting of only one resonance
(c) D possesses a $^1H$ NMR spectrum consisting of two signals in the ratio 1:3
(d) Two singlets would be observed in the $^1H$ NMR spectrum of D
(e) B and C both possess $^1H$ NMR spectra containing a singlet, a triplet and a quartet
(f) The $^1H$ NMR spectrum below belongs to B:

3. There are three sets of equivalent $^1H$ atoms bonded to carbon in paracetamol:
• (A) corresponds to the three equivalent $^1$H on a -CH$_3$ group. These are expected to have a chemical shift of 0.8 – 1.8 ppm. As it is due to three $^1$H, the signal will have a relative area of 3.

• (B) corresponds to two equivalent $^1$H on the ring. These are expected to have a chemical shift of 6 – 9 ppm. As it is due to two $^1$H, the signal will have a relative area of 2.

• (C) correspond to another two equivalent $^1$H on the ring. These are expected also to have a chemical shift of 6 – 9 ppm. As it is due to two $^1$H, the signal will have a relative area of 2.

• The chemical shifts of {C} will be different to those of {B} but you are not expected to order them.

Each proton in {B} is adjacent to one proton from set {C} and coupling will split the signal due to the {B} protons into a doublet.

Each proton in {C} is adjacent to one proton from set {B} and coupling will similarly split the signal due to the {C} protons into a doublet.

The $^1$H NMR spectrum due to the protons bonded to carbon will thus consist of three signals (due to A, B and C) and the signals due to B and C will be doublets.

\[ \text{2-methylpropan-1-ol} + \text{Cr}_2\text{O}_7^{2-} / \text{H}^+ \rightarrow \text{isobutyric acid} \]

$1^\circ$ alcohol $\rightarrow$ carboxylic acid
butan-2-ol $\xrightarrow{\text{Cr}_2\text{O}_7^{2-}/H^+}$ butan-2-one

$\text{2° alcohol} \rightarrow \text{ketone}$

2-methylpropan-2-ol $\xrightarrow{\text{Cr}_2\text{O}_7^{2-}/H^+}$ No reaction

$\text{3° alcohol} - \text{no reaction with oxidizing agent}$

2-methylpropan-2-ol $\xrightarrow{\text{H}_2\text{SO}_4}$ 2-methylprop-1-ene

Dehydration of 3° alcohol

2-methylprop-1-ene $\xrightarrow{\text{H}_2\text{SO}_4}$ 2-methylpropan-2-ol

Hydration of a C=C bond

See the ‘Organic Spectroscopy’ website for more information and practice: