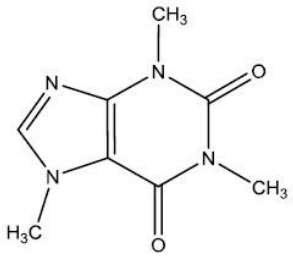
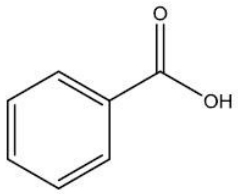
Problem 8: Compound confusion

Pre-Lab answers

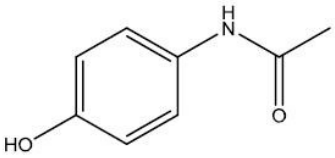
1.



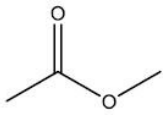
caffeine, m.p. 238 °C



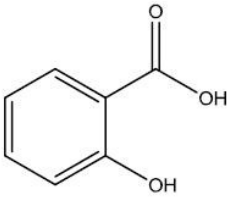
benzoic acid, m.p. 122 °C



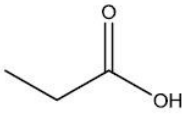
paracetamol, m.p. 170 °C



methyl ethanoate, m.p. – 98 °C



2-hydroxybenzoic acid, m.p. 159 °C



propanoic acid, m.p. –21 °C

2.

A pure compound will melt over a relatively narrow temperature range. Impurities both lower the temperature at which the compound melts and widens the range over which it melts.

3.

For benzoic acid;

$$C_6H_5COOH + NaHCO_3 \rightarrow C_6H_5COO^-Na^+ + H_2O + CO_2$$
$$2\ C_6H_5COOH + Na_2CO_3 \rightarrow 2\ C_6H_5COO^-Na^+ + H_2O + CO_2$$

For 2-hydroxybenzoic acid;

$$C_6H_5(OH)COOH + NaHCO_3 \rightarrow C_6H_5(OH)COO^-Na^+ + H_2O + CO_2$$
$$2\ C_6H_5(OH)COOH + Na_2CO_3 \rightarrow 2\ C_6H_5(OH)COO^-Na^+ + H_2O + CO_2$$

For propanoic acid;

$$C_2H_5COOH + NaHCO_3 \rightarrow C_2H_5COO^-Na^+ + H_2O + CO_2$$
$$2\ C_2H_5COOH + Na_2CO_3 \rightarrow 2\ C_2H_5COO^-Na^+ + H_2O + CO_2$$

4.

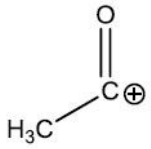
a) A deuterium atom is an isotope of hydrogen with atomic mass 2 (1 proton, 1 neutron, 1 electron)

b) The residual solvent peak is a result of the small quantities of $CHCl_3$ or $(CH_3)_2SO_2$ present in the bottles of the deuterated solvents.

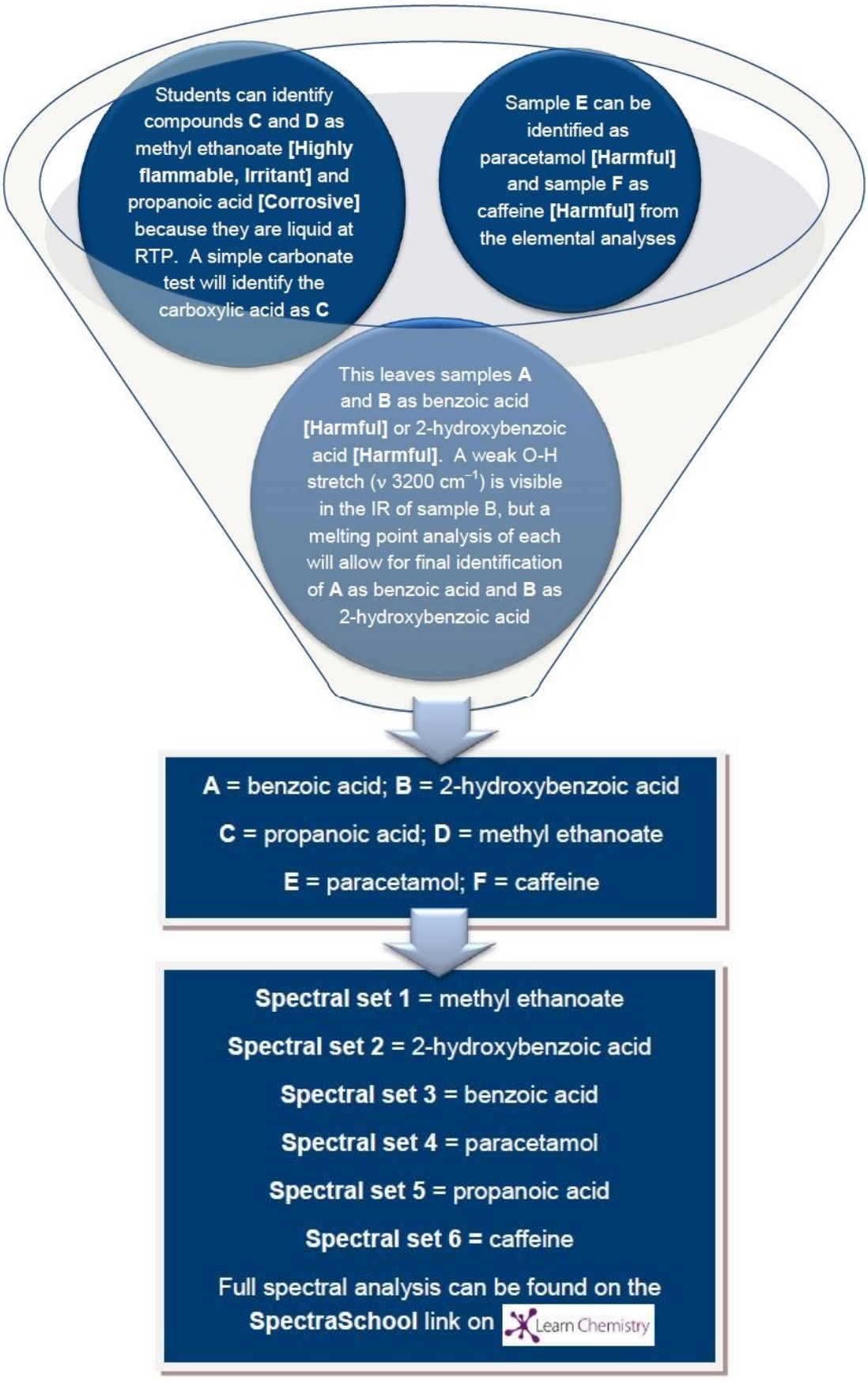
c) $CDCl_3$ Residual solvent peak in ^{13}C NMR – δC 77.2 ppm, triplet
DMSO Residual solvent peak in ^{13}C NMR – δC 39.5 ppm, septuplet

5.

m/z 43 = acylium ion



$$[HOC_6H_4NHC(O)CH_3]^{+\bullet} \rightarrow [CH_3C(O)]^{+} + [HOC_6H_4NH]^{\bullet}$$



Equipment list

Each group will need;

- Small samples of each of the compounds labelled A – F
- benzoic acid **[Harmful]** labelled *Sample A*
- 2-hydroxybenzoic acid **[Harmful]** labelled *Sample B*
- propanoic acid **[Corrosive]** labelled *Sample C*
- methyl ethanoate **[Highly flammable; Irritant]** labelled *Sample D*
- paracetamol **[Harmful]** labelled *Sample E*
- caffeine **[Harmful]** labelled *Sample F*
- Access to a melting point apparatus
- Melting point tubes
- Test tubes
- Sodium carbonate **[Irritant]** or sodium hydrogen carbonate **[Low hazard]**
- Spatula
- Disposable pipettes
- Universal Indicator solution