# TOPIC 20 EXERCISE 2 – CARBON-13 NMR SPECTRA

1. a) Suggest how propanal and propanone could be distinguished from their carbon-13 nmr spectra.

    b) Suggest how propan-2-ol and propanone could be distinguished from their carbon-13 nmr spectra.

    c) Predict the number of peaks in the carbon-13 nmr spectrum of:
        i)   butanone
        ii)   pentan-2-one
        iii) pentan-3-one

2. Can you find seven different molecules which could be responsible for the carbon-13 nmr spectrum below? (rmm = 116)

CDS-00-750
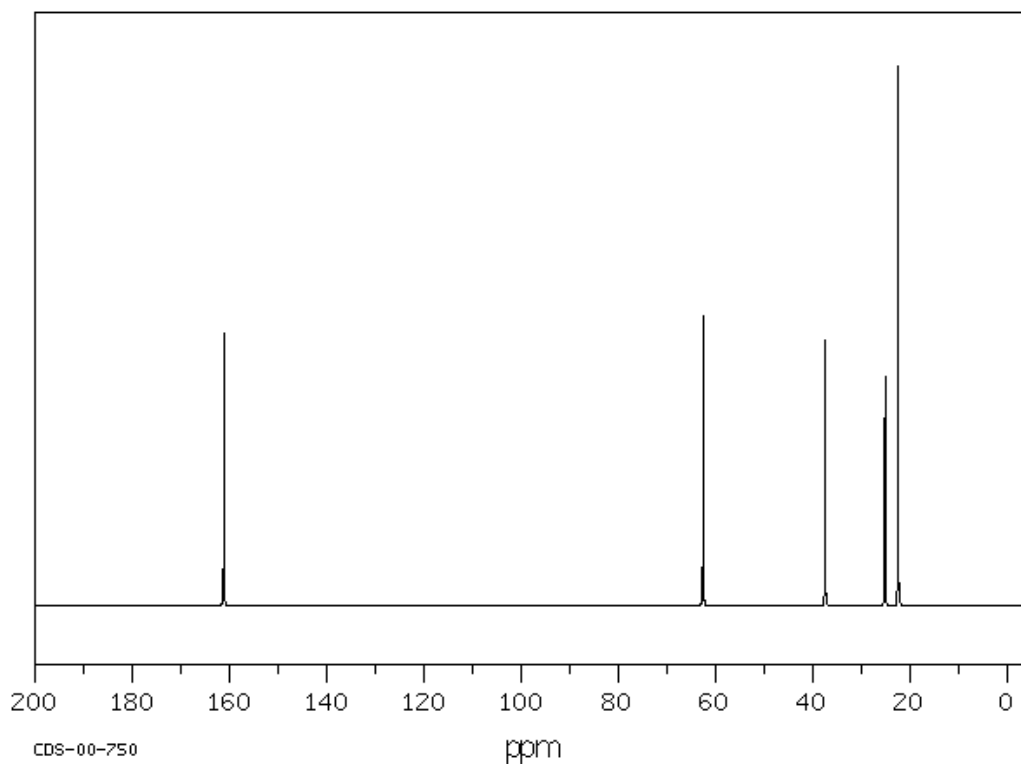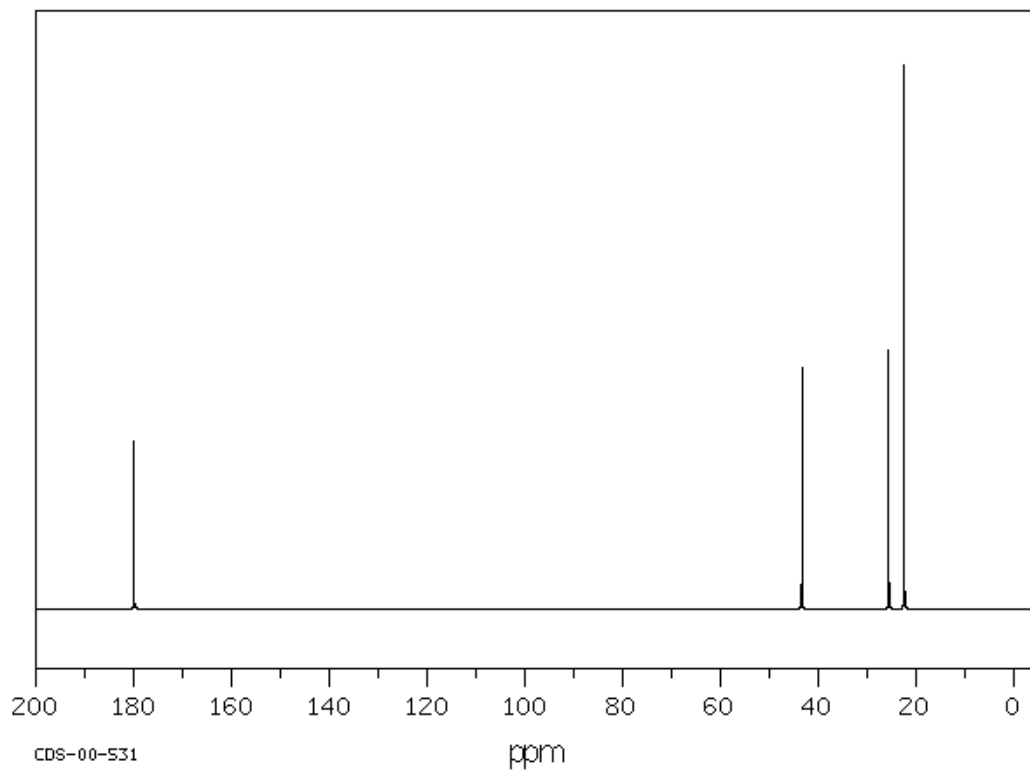
3. Can you identify this molecule (rmm = 74)?

CDS-03-913

ppm
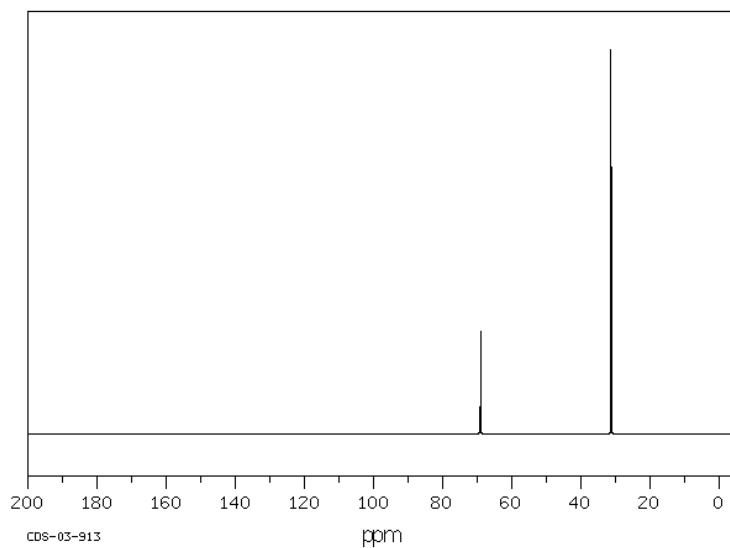
4. Can you find three possible structures for this molecule (rmm = 86)?

CDS-03-859

ppm
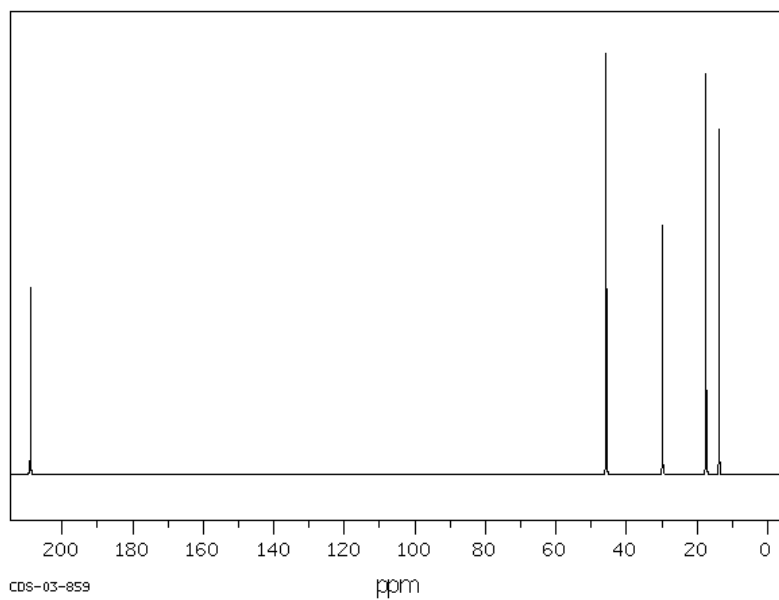
5. Can you identify this molecule (rmm = 102)

CDS-00-531

ppm

SOLUTIONS

1.   a)   Propanal has three peaks, propanone has two
        b)   Both have two peaks, one with chemical shift between 0 and 50. However the second peak in propanone will have a chemical shift at 160 – 220, but the second peak in propan-2-ol will have a chemical shift at 50 - 90
        c)   i) 4   ii) 5   iii) 3

2.   Peak at 60 ppm C-O and peak at 160 ppm O=C-O so ester is most likely
$C_nH_{2n}O_2 = 116$ so $n = 6$

Five peaks so two C atoms are in identical environments, likely $-C(CH_3)_2$
$HCOOCH_2CH_2CH(CH_3)_2$ or $HCOOCH(CH_3)CH(CH_3)_2$ or
$CH_3COOCH_2CH(CH_3)_2$ or $CH_3CH_2COOCH(CH_3)_2$ or
$(CH_3)_2CHCOOCH_2CH_2CH_3$ or $(CH_3)_2CHCOOCH_2CH_3$ or
$(CH_3)_2CHCH_2COOCH_3$

3.   Peak at 60 ppm C-O so alcohol is most likely
$C_nH_{2n+2}O = 74$ so $n = 4$
Two peaks so three C atoms are in identical environments, likely $-(CH_3)_3$
$(CH_3)_3COH$

4.   Peak at 210 ppm = C=O so carbonyl most likely
$C_nH_{2n}O = 84$ so $n = 5$
Five peaks so no C atoms in identical environments
$CH_3CH_2CH_2CH_2CHO$ or $CH_3CH_2CH(CH_3)CHO$ or $CH_3CH_2CH_2COCH_3$

5.   Peak at 180 ppm = O=C-O so carboxylic acid most likely
$C_nH_{2n}O_2 = 102$ so $n = 5$
Four peaks so two C atoms in identical environments, likely $-C(CH_3)_2$
$(CH_3)_2CHCH_2COOH$