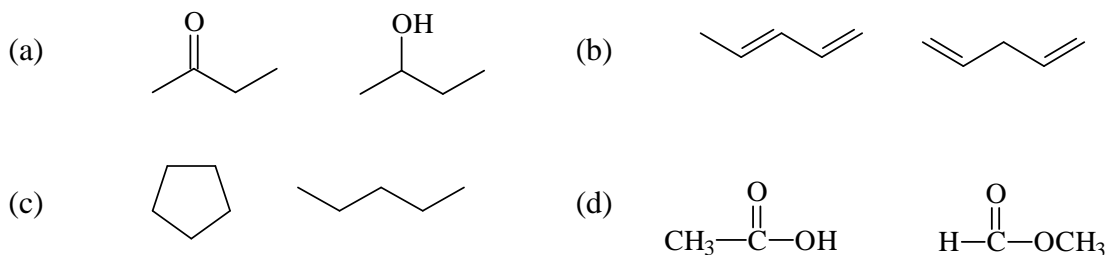




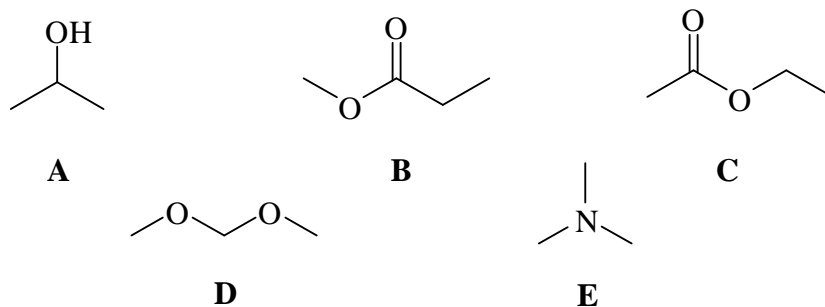
Problem Sheet 2

1. Low resolution mass spectrometry indicated a molecular ion at $m/z = 58$. The compound could be C_3H_6O or C_4H_{10} or $C_2H_6N_2$. High resolution mass spectrometry gave a value of $m/z = 58.0530$. Using the following more accurate atomic weight data determine which compound it is.
Data: 1H 1.0078; ^{14}N 14.0031; ^{12}C 12.0000; ^{16}O 15.9949

2. Which spectroscopic technique would most readily distinguish between the following pairs of compounds? Give a brief reason.



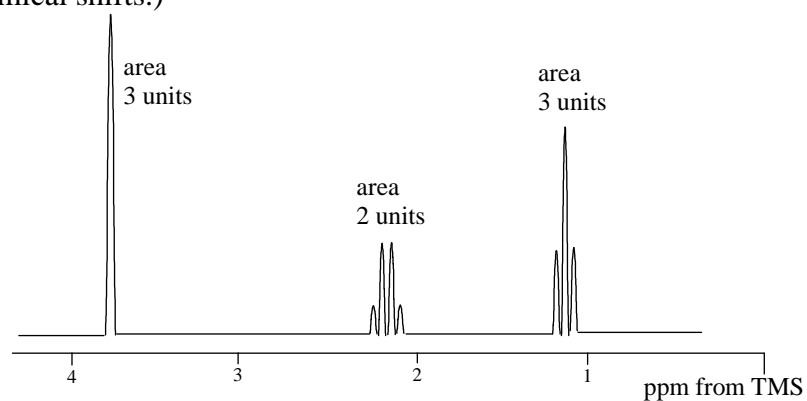
3. Consider the following molecules, **A** - **E**.



More than one answer may be correct. Give all correct answers.

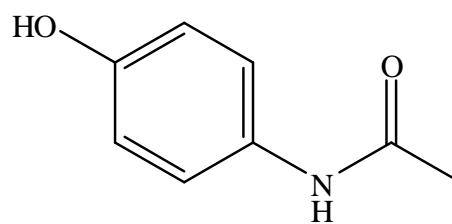
- (a) Which of the molecules would give three signals in the 1H NMR spectrum?
(b) Which of the molecules would possess a 1H NMR spectrum consisting of only one resonance?
(c) Which of the molecules would possess a 1H NMR spectrum consisting of two signals in the ratio 1:3?
(d) How many singlets would be observed in the 1H NMR spectrum of **D**?
(e) Which of the molecules would possess a 1H NMR spectrum containing a singlet, a triplet and a quartet signal?

- (f) Examine the ^1H NMR spectrum below. To which of the compounds does it belong? (Hint: See page E35-11 of the Laboratory Handbook for approximate chemical shifts.)



4. By first considering the number and type of ^1H environments, *sketch* the ^1H NMR spectra you would expect for paracetamol. You only need to consider the protons bonded to carbon.

Your diagram should include coupling patterns and integration of each multiplet.

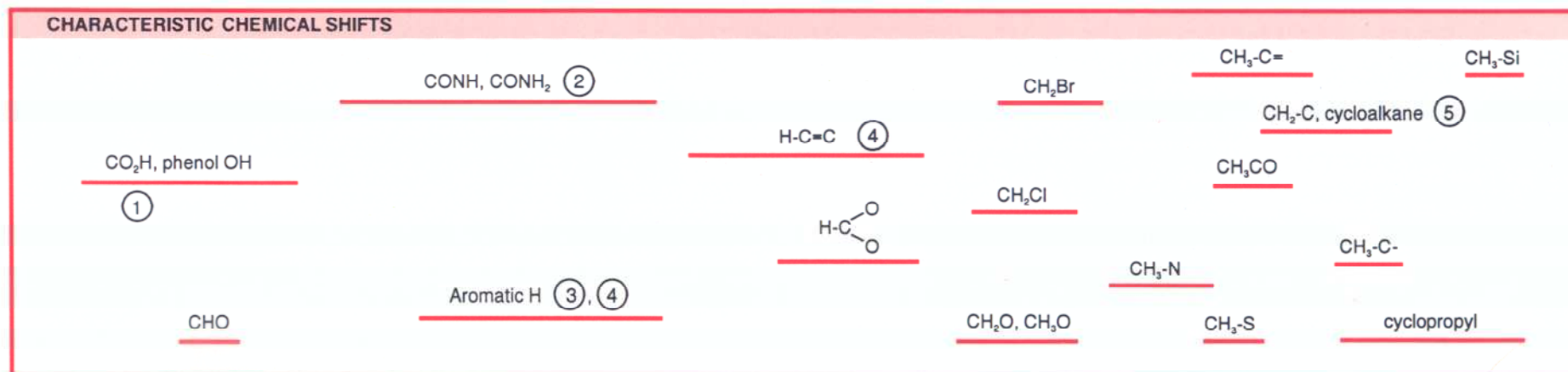
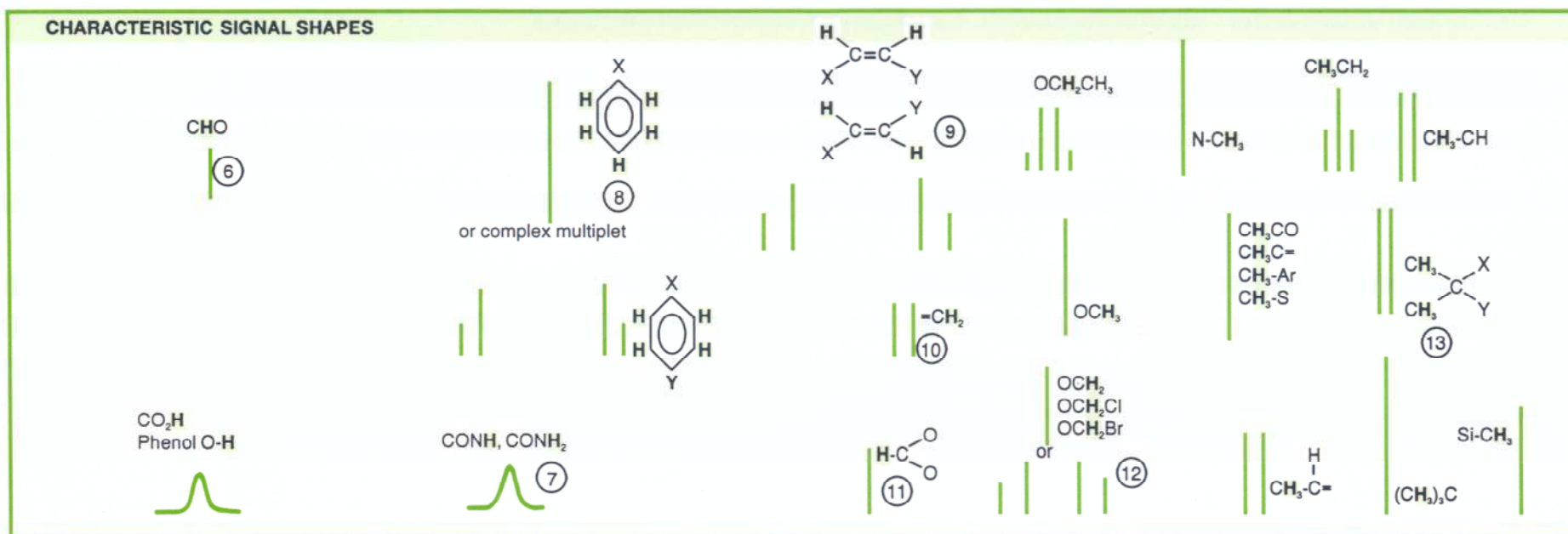


paracetamol

(Hint: Use the table on the next page to find out the approximate chemical shifts.)

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¹H NMR Spectral Characteristics



LOW FIELD 8 10 9 8 7 6 5 4 3 2 1 0 HIGH FIELD

KEY Upper part shows characteristic shapes of various signals and lower part gives region of NMR spectrum where they may be found

USE Use lower part for the possible origin of signals in your spectrum then refer to upper part for distinguishing features. N^m in circles refer to key overleaf