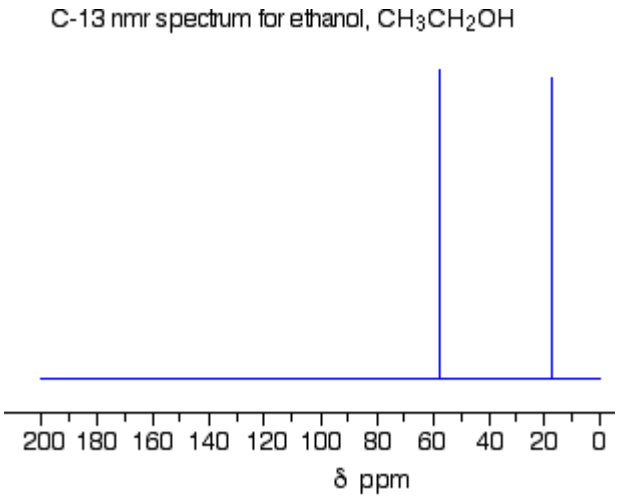
C-13 NMR: INTRODUCTION

1. Carbon-13 atoms have a nucleus which can behave as a tiny magnet which will align with an external magnetic field. If you pass energy in the form of radio waves with a frequency of about 25 MHz through a carbon-containing substance, for a particular magnetic field, the C-13 nuclei will flip constantly backwards and forwards from being aligned with the field to being aligned against it. This is known as the resonance condition, and can be detected and displayed on a C-13 NMR spectrum.

   a) The environment around each carbon atom is important. Explain carefully why the two carbon atoms in ethanol, CH_3CH_2OH would need different magnetic fields to achieve resonance for a particular frequency of radio waves.

   The C-13 NMR spectrum for ethanol looks like this:



   b) The standard for comparison which gives a peak at 0 (often left out when these spectra are drawn) is called TMS. What does TMS stand for? Draw the structure of the molecule.

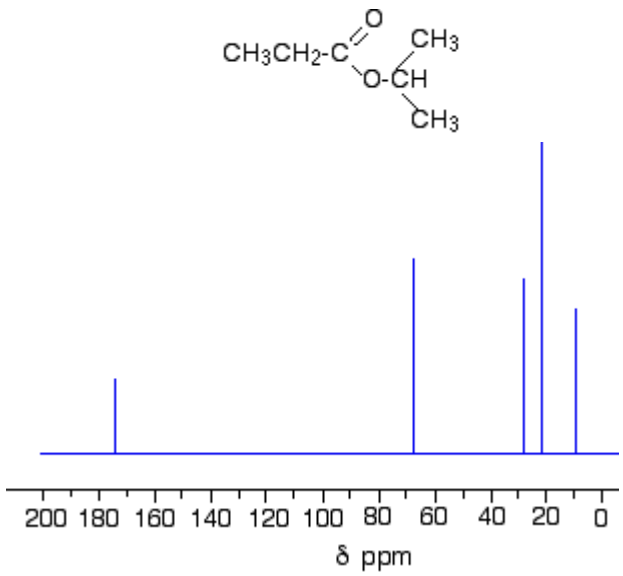
   c) The horizontal scale on these spectra is in terms of "ppm" - parts per million. Explain what that means by considering the position of the right-hand one of the two peaks.

   d) Explain briefly why TMS is chosen as the standard.

   e) Considering the environments of the two carbons in ethanol, which one do you think will have given the right-hand peak, and which the left-hand one? Explain your reasoning.

questions continue. . .

2. a) The spectrum below is for the compound 1-methylethyl propanoate which has the structure:



Explain carefully why the spectrum has five peaks. (You aren't expected to decide which peak is which.)

b) How many peaks would you expect to find in the C-13 NMR spectrum for

(i) pentan-3-one, $CH_3CH_2COCH_2CH_3$

(ii) pentan-2-one, $CH_3CH_2CH_2COCH_3$?