Chemguide – answers

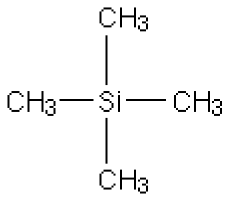
H-1 NMR: INTRODUCTION

1. a) Think about the electrons around each hydrogen atom. If an atom has electron pairs close to its nucleus, these shield it to some extent from the magnetic field. The closer they are, the more the nucleus is shielded.

   A hydrogen atom bonded to an electronegative oxygen atom has the bonding pair of electrons pulled away from itself, compared with what happens when it is attached to a carbon atom. If you keep the frequency of the radio waves the same, hydrogens in different environments cannot come into the resonance condition with the same external magnetic field, because the field they are actually experiencing is slightly different.

   To compensate for the greater shielding, you would have to increase the external magnetic field slightly for the hydrogen which isn't attached to the oxygen.

   b)



   All the hydrogen atoms in TMS are in exactly the same environment, and so will only produce a single peak. There are also 12 of them, so the peak is likely to be strong and easily visible.

   The electrons in TMS lie more closely to the hydrogen atoms than in almost any other organic compound, and so these hydrogen atoms are the most shielded from an external magnetic field. That means that you will need a higher external magnetic field in this compound than in almost any other to bring the hydrogen nuclei into resonance. That places the peak at the extreme right-hand side of the spectrum.

2. a) This is because all the hydrogen atoms in the compound are in exactly the same environment. The two CH_3 groups are exactly equivalent.

   b) According to SDBS (the source of these spectra), the peak is at 3.242 ppm. That means that the external magnetic field needed to bring these hydrogens into the resonance condition is 3.242 millionths less than the one needed for the hydrogens in TMS.

   c) The three clusters of peaks are because the hydrogen atoms are in three different environments. This is obvious from the formula, CH_3CH_2OH. Electron shifts in the molecule (due mainly to the electronegativity of the oxygen) mean that the OH hydrogen and the CH_2 hydrogens and the CH_3 hydrogens will all experience slightly different amounts of shielding from the external magnetic field.

   The areas under the peaks give a count of the number of hydrogens in each environment. If the areas are in the ratio 2 : 1 : 3, then the cluster of peaks at just under 4 ppm must be due to the CH_2 group hydrogens; the single peak must be due to the OH hydrogen; and the cluster on the right due to the CH_3 hydrogens.

d) (i) pentan-3-one, $CH_3CH_2COCH_2CH_3$: 2. The CH_2 groups are both in identical positions and so are the CH_3 groups.

(ii) pentan-2-one, $CH_3CH_2CH_2COCH_3$: 4. There are no two groups in *exactly* the same environment. One of the CH_3 groups is very near an oxygen atom; the other more distant from it. Similarly with the CH_2 groups. Nearness to an oxygen atom matters because its high electronegativity pulls electron pairs towards itself, and that effect is felt less and less the farther away you get from the oxygen.