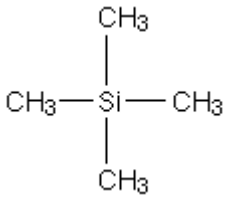
C-13 NMR: INTRODUCTION

1. a) You have to think about the electrons around each carbon 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.

   One of the carbons is bonded to an electronegative oxygen atom which pulls the bonding pair towards itself, and that will reduce the shielding compared with the other carbon atom. If you keep the frequency of the radio waves the same, both of the carbons 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 use a slightly higher magnetic field with the carbon not attached to the oxygen.

   b) Tetramethylsilane 

   c) Suppose the right-hand peak is at about 18 ppm. This means that the magnetic field needed to bring this carbon into the resonance condition is 18 millionths less than the field needed for the carbon atoms in TMS.

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

   The electrons in TMS lie more closely to the carbon atoms than in almost any other carbon compound, and so these carbon 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 carbon nuclei into resonance. That places the peak at the extreme right-hand side of the spectrum.

   e) The carbon attached to the oxygen has the smaller amount of shielding because the oxygen pulls electrons away from it. That means that the external field needed will be less than in the case of the CH_3 carbon atom - we have already talked about this in part (a). So how does this fit onto the diagram compared with TMS?

   TMS will need the greatest external field because its carbon nuclei are the most shielded. The carbon nucleus in the CH_3 group isn't shielded quite as much and so needs a field about 18 millionths less than TMS. The CH_2 carbon is even less shielded, and so needs an external field of only about 60 millionths less than TMS. So the CH_2 carbon gives the left-hand peak, and the CH_3 the right-hand one.

   (It is good for you to be able to think this through, but in most cases you will meet, it probably won't be necessary - as you will find in the next page in this section about C-13 NMR.)

2. a) This shows that there are carbon atoms in 5 different environments. However there are 6 carbons in total, and so 2 of them must be in completely identical environments. Those two are the two CH_3 groups on the right-hand side of the molecule.

The CH_3 group on the left-hand side isn't in exactly the same environment. Although it is also attached to 3 hydrogens and another carbon, the environment isn't *identical*, because what happens further along the chain isn't exactly the same.

b) (i) 3. There is the carbon atom in the C=O bond and the two carbons in the CH_3CH_2 groups. Both CH_3 carbons are in identical environments, as are both CH_2 carbons. (Talk yourself along the chain if you aren't convinced: "The left-hand CH_3 carbon is attached to a CH_2 carbon which is attached to . . ." and then do it again from the other end. Similarly for the CH_2 carbon.)

(ii) 5. None of the carbon atoms are in identical environments. Talk yourself along the chain if you need to.