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CHEM 3420: Physical Chemistry II — Spring 2009

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Lecture 29: NMR Spectroscopy

References

1. Levine, *Physical Chemistry*, Section 20.12

Key Concepts

- Some nuclei, like ^{1}H, have two intrinsic spin states, up and down. Under an applied magnetic field, these two states have different energies.
- It is possible to probe the transition between these two states through absorption spectroscopy. The transition frequency is typically in the MHz or radio frequency range of the spectrum. The magnetic field necessary to observe the transition varies between 1.5 T and 15 T.
- The stronger the magnetic field, the larger the energy difference between the two spin states, and the larger frequency of absorption.
- It is possible to measure the spectrum in two ways:
  1. Fix the magnetic field and vary the the frequency to find absorption (when $\Delta E = h\nu$).
  2. Fix the frequency and vary the magnetic field to find absorption.
- The local environment of an atom impacts its behavior in a magnetic field. If there are many electron withdrawing atoms in the vicinity, then atom of interest is said to be de-shielded. The reduction of electron density around the nucleus results in a larger ΔE and thus a larger absorption frequency, i.e. the peak will be downshifted (large chemical shift).
- There is also coupling between protons (^{1}H) since they are not isolated. This coupling generally manifests itself as the appearance of multiplets of peaks as opposed to a single peak.
- If there are n equivalent neighboring protons to a particular proton of interest, then there are $n + 1$ peaks associated with the proton of interest. This is due to the multiplicity of spin states of the neighboring protons. If there are two identical neighbors, there are 3 possible spin states and thus three peaks arise due to the interactions.

Related Exercises in Levine

Exercises 20.25, 20.26