What is NMR Spectroscopy?

Worksheet

NMR works by aligning atomic nuclei in a magnetic field, then detecting the radiofrequency energy they absorb and emit. Chemical shift () tells where atoms sit in a molecule; spin-spin coupling shows how many neighbors they have.

Questions

1. A peak in H NMR at = 9.8 ppm is most likely

A) An aldehyde proton (CHO)
B) A methyl group (CH)
C) A methylene group (CH)
D) An aromatic proton

2. In the H NMR of propane (CHCHCH), what is the coupling pattern for the central CH?

A) Singlet
B) Doublet
C) Quartet
D) Septet

3. What does a triplet in H NMR indicate?

A) Three protons in the same environment
B) Coupling to 2 neighboring equivalent protons
C) Three peaks for one type of proton
D) An aromatic compound

4. C NMR typically shows peaks at higher values than H NMR because

A) Carbon nuclei are larger
B) C nuclei are more easily shielded
C) C nuclei are more strongly deshielded by electron density changes
D) C requires higher radiofrequency

5. A proton in a benzene ring appears at 7.3 ppm. What does this tell you?

6. An ethanol (CHCHOH) H NMR shows two triplets and a quartet. Explain.

7. In an NMR spectrum, peak A has twice the area of peak B. What does this mean?

8. Define: What does chemical shift () measure?

9. Define: What causes spin-spin coupling?

10. Define: What is the reference standard for H NMR?

Answer Key

1. A) An aldehyde proton (CHO) - Aldehyde protons are highly deshielded and appear at = 9-10 ppm. Methyl/methylene appear at 0-2 ppm; aromatics at 7-8 ppm.

2. D) Septet - The central CH is surrounded by 6 equivalent H (two CH groups), so it couples to n=6, giving a septet (6+1=7 lines).

3. B) Coupling to 2 neighboring equivalent protons - A triplet (three lines) means n+1=3, so n=2 neighboring equivalent protons. This is the n+1 splitting rule.

4. C) C nuclei are more strongly deshielded by electron density changes - Carbon nuclei are much more sensitive to changes in local electron density than protons, so they show a larger range of chemical shifts (0-200+ ppm for C).

5. The chemical shift of 7.3 ppm is typical of aromatic (benzene-ring) protons. This chemical shift range indicates the proton is shielded by the -electron cloud of the ring. We can confidently assign this peak to aromatic protons, not aliphatic (alkyl) protons.

6. The CH (methyl) group couples to 2 neighboring H on CH gives a triplet. The CH group couples to 3 neighboring H on CH gives a quartet. The OH proton often exchanges rapidly and does not show coupling. This pattern is called an ethyl (Et) group signature.

7. Peak area (integration) is proportional to the number of protons. If A is twice the area of B, then A represents twice as many equivalent protons as B. Example: a methyl group (3H) will have an area 1.5 larger than a methine (2H).

8. The position of a peak in an NMR spectrum, measured in parts per million (ppm) relative to a reference (TMS). It reveals the local electronic environment of a nucleus.

9. Magnetic interaction between neighboring nuclei. Nuclei with n neighbors split into n+1 peaks (doublet, triplet, quartet, etc.).

10. Tetramethylsilane (TMS) at = 0 ppm. All other peaks are measured relative to TMS.