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NMR Theory

Transcript

00:00:01:56 - 00:00:11:84
Dr.Jessie Key: Hello again, Dr. Jessie Key here. In this video, we're going to discuss Nuclear Magnetic Resonance Theory as it pertains to Carbon NMR.

00:00:11:88 - 00:00:39:71
Dr.Jessie Key: Nuclear Magnetic Resonance (NMR) spectroscopy is super important because it is arguably the most powerful method of gaining structural information about organic compounds. NMR involves an interaction between electromagnetic radiation and the nucleus of an atom. A nucleus with an odd number of protons or an odd number of neutrons possesses the quantum mechanical property of nuclear spin.

00:00:39:71 - 00:01:04:21
Dr.Jessie Key: Spinning charge in the nucleus creates a magnetic moment, a magnetic field similar to the magnetic field produced by a bar magnet. In the absence of an externally applied magnetic field, magnetic moments of nuclei are disordered. However, upon the application of an external magnetic field, abbreviated here as B naught, the magnetic moments will align.

00:01:04:21 - 00:01:18:09
Dr.Jessie Key: Magnetic moments can be aligned with external magnetic field. This is called the alpha spin state. Or they can be aligned against the external magnetic field, which is called the Beta spin state.

00:01:18:09 - 00:01:46:46
Dr.Jessie Key: The Alpha α and Beta β spin states are not equal in energy, it is higher energy to be aligned against the magnetic field. The stronger the magnetic field, the greater the energy gap that exists between the Alpha and Beta spin states. Nuclei can be excited from the lower energy Alpha state to the higher energy Beta state by absorption of a pulse of radio frequency energy.

00:01:46:46 - 00:02:11:05
Dr.Jessie Key: This transfer of energy and excitation is called resonance. The signal that we observe results from the corresponding relaxation and release of energy by individual

nuclei. The combination of multiple frequencies of electromagnetic radiation emitted by the sample's nuclei is known as a “Free Induction Decay” (or FID for short).

00:02:11:05 - 00:02:43:71
Dr.Jessie Key: We can use computer processing software and mathematics known as a Fourier Transform, to convert the FID to an interpretable NMR spectrum. In modern NMR instruments, a sample tube is placed in the presence of a strong magnet as shown in the center of the image. A radio frequency generator shown bottom left is used to excite nuclei from the lower energy Alpha state to the higher energy Beta state with a broad pulse of radio frequencies.

00:02:43:80 - 00:03:15:93
Dr.Jessie Key: The detector and amplifier shown bottom right later detects the energy released upon relaxation to lower energy Alpha state and amplifies a signal, which is then passed on to the computer for processing. The image on this slide is of a modern Fourier transform NMR, which has been cut in half for educational purposes. Special thanks go to the University of Alberta Department of Chemistry NMR Services, who have graciously permitted me to use this image and who also supported me during my PhD.

00:03:15:93 - 00:03:38:73
Dr.Jessie Key: Samples are placed in plastic spinner adapters and put into the top of the instrument the sample port. The outer layer of the instrument is composed of reflective Mylar and vacuum sealed for insulation. As we move further in, there is a liquid nitrogen reservoir at approximately 77 Kelvin, which serves as the first layer of refrigerant.

00:03:38:73 - 00:04:08:94
Dr.Jessie Key: Next, there's another layer of reflective Mylar and vacuum sealed for insulation, followed by a liquid helium reservoir at approximately 4 Kelvin as the second layer of refrigerant. The orange-coloured solenoid magnet is made of superconducting wire of fine strands of a tin-niobium-tantalum alloy coated in a copper matrix. Further within the instrument is the probe which contains receiver coils to detect the signal.

00:04:08:94 - 00:04:34:72
Dr.Jessie Key: The first NMR spectrometers were developed in the 1950's. They're often referred to as Continuous-wave or CW NMR instruments because they operated very differently than current instruments by continuously changing the magnetic field strength instead of changing the radio frequency. Shown on the left is a photograph of a NMR spectrometer from the year 1957 with its operator.

00:04:34:73 - 00:04:52:25
Dr.Jessie Key: Shown on the right is a photograph of a very modern 900MHz megahertz NMR instrument located at the University of Ottawa. Notice this instrument is so large that stairs and a platform are built to allow the operator to reach the sample port at the top.