

Very Short Appendix of Basic Chemistry and Physics

The subjects covered in this appendix fill whole chapters of general chemistry and general physics texts; if the treatment below is too abbreviated for you then please refer to such texts.

CHEMISTRY

Atomic Numbers and Mass Numbers.

The atomic number of an element is the number of protons in its nucleus, denoted Z . The mass number is the sum of protons (Z) and neutrons (N), $M = Z + N$. A shorthand for the number of Z and M is to show the M as superscript and the Z as subscript, ${}^M_Z\text{E}$. Different isotopes of the same element have the same Z , but different N and thus different M .

“Rules” for Electrons in Orbitals

The Pauli Exclusion Principle says that no two electrons in an atom can have the same four quantum numbers (n, l, m_l, m_s). Since electrons have spin $m_s = +1/2$ or $-1/2$, what this means is that only two electrons can occur in an orbital, and they must have antiparallel spins. Hund’s rule says that electrons will occur singly in degenerate orbitals with parallel spins before any of these orbitals has paired electrons.

Bonding orbitals are formed by combination of atomic orbitals of the two atoms involved. Hybrid orbitals, generally sp^x ($x = 1, 2, 3$) for the molecules considered in BCM 230, are formed by combination of atomic orbitals. While p orbitals have a node at the nucleus, s orbitals actually have large electron density at the nucleus. Only s orbitals or hybrid orbitals with s character are important for spin-spin coupling (see text) since only these orbitals have electron density at the nucleus.

PHYSICS

Vectors

A vector possesses both magnitude and direction. Vectors are represented by arrows, with length proportional to magnitude. \longrightarrow Vectors are often denoted with bold type or with a half arrow: \mathbf{a} \vec{a}

Vectors can be added. The vector sum of \uparrow and \rightarrow is \nearrow . The vector sum of \uparrow and \downarrow is zero. The component vectors must be of the same kind. An example is individual magnetizations \mathbf{m}_i summing to form the bulk magnetization \mathbf{M} .

Vectors of different kinds can be multiplied together in two ways: the scalar or dot product and the vector or cross product. In NMR, the cross product is usually what concerns us. The vector (cross) product of vectors \mathbf{a} and \mathbf{b} is written :

$$\mathbf{a} \times \mathbf{b} = \mathbf{c}$$

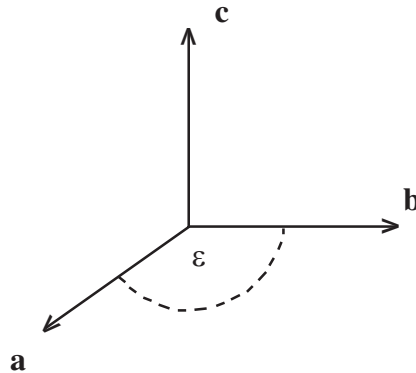
where \mathbf{c} is the resultant vector. An example in NMR of cross product vector multiplication is the \mathbf{B}_1 field acting on the bulk magnetization \mathbf{M} .

The magnitude of \mathbf{c} is given by:

$$c = (ab)\sin(\varepsilon)$$

where ε is the angle between \mathbf{a} and \mathbf{b} and a, b are the magnitudes of the vectors.

The direction of \mathbf{c} is defined to be in a plane perpendicular to the plane formed by \mathbf{a} and \mathbf{b} (the “right hand rule”).

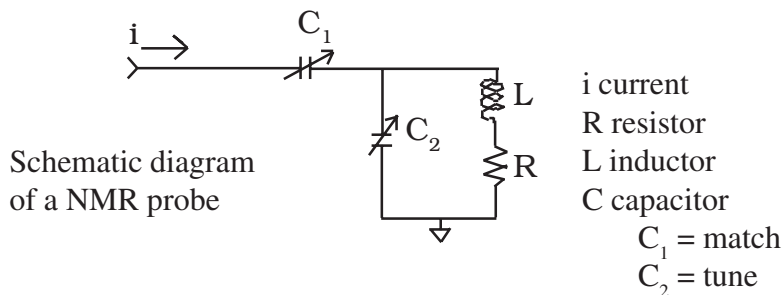


Maxwell's Equations

Maxwell's equations summarize many basic properties of electromagnetism. The two that particularly apply to NMR are Ampere's Law (as extended by Maxwell) and Faraday's Law of Induction. The former tells us that *a current in a wire produces a magnetic field near the wire*. The latter says that *a bar magnet, thrust into a closed loop of wire, will set up a current in the loop*. The specific equations are presented in any general physics text.

Circuits; Probe tuning

An NMR probe, in essence, is a tuned circuit much like you would find in a radio. There are many ways to build a tuned circuit, the most common of which is the parallel resonant configuration shown here.



The inductor L is the NMR coil and C_2 is the variable tuning capacitor. The resonance condition at frequency f is achieved when

$$(2\pi f)^2 LC_2 = 1$$

To tune the probe to the correct Larmor frequency ($f = \omega_L$) C_2 is varied until the resonance condition is achieved.

R in the probe diagram is the combined resistance of the wire that forms the coil and the connections between the circuit elements. R is important as it affects the Q of the circuit where

$$Q = 2\pi fL/R$$

Q is a measure of probe performance. Higher Q means a more sensitive probe (it produces higher signal-to-noise), so NMR engineers try to make R as small as possible and L as large as possible. However, there are limits on L imposed by the equation $(2\pi f)^2 LC_2 = 1$ and the choice of variable capacitors available (normally 1 – 30 picofarad).

The variable capacitor C_1 in the probe diagram is called the coupling or match capacitor. Its purpose is to impedance match the circuit. Maximum power transfer is achieved when the load impedance (the tuned probe circuit) is the same as the source impedance (the high power amplifier that produces the pulse). In NMR the standard source impedance is 50 ohms resistive. Thus C_1 is changed until the probe circuit looks 50 ohms resistive.

The NMR spectrometer comes with hardware and software that enables one to easily (usually) tune the probe to the Larmor frequency and impedance match it as well; the combined procedure is usually called “probe tuning”.

In principle, changing the match should not affect the tune and vice versa. However, the reality is that they do. Thus, probe tuning is an iterative procedure using C_1 and C_2 until the probe is tuned and matched properly.