Exam 1: CHEM/BCMB 4190/6190/8189 (136 points) Thursday, 8 September, 2022

1). There are two contributors to the NMR relaxation parameter T_2^*. Please identify these contributors and their origins, and how they contribute, microscopically, to relaxation in the transverse plane. (**8 points**)

Magnetic field inhomogeneity is the first contributor. For bulk magnetization in the transverse plane, the precession frequencies of the individual magnetic dipoles that comprise the ensemble are dependent on the magnitude of the field strength that each experiences. As the static magnetic field, B_0, becomes less homogeneous, the range of precession frequencies increases, and the individual magnetic dipoles diverge from one another faster, destroying the phase coherence in the transverse plane and decreasing the amplitude of the observed signal.

The second contributor is spin-spin relaxation or the "true" T_2 component. The individual nuclear dipoles reorient randomly creating local electromagnetic fields that either augment or oppose B_0. As with magnetic field inhomogeneity, because the precession frequencies depend on the effective field strength experienced by each nucleus, the range of precession frequencies increases, which, again, results in loss of phase coherence in the transverse plane.

2). The Larmor frequency for ^1H is 400 MHz in a magnet with a magnetic field strength of 9.4 T. What would be the magnetic field strength of a magnet that would make the Larmor frequency of this nucleus 900 MHz? (**4 points**)

Larmor frequency is directly (linearly) dependent on magnetic field strength. If the Larmor frequency is increasing by a factor of 2.25 (i.e., 900/400=2.25), then this means that the magnetic field strength increased by this factor as well. So, 9.4 T x 2.25 = 21.1 T.

3). For a compound with a single ^1H nucleus (i.e. $CHCl_3$), following a 90° ^1H pulse along the +x-axis, the bulk ^1H magnetization vector lies along the y axis in the transverse plane, as shown in 'A' below. In the *rotating frame*, after a short time, the bulk magnetization vector has moved to the position shown in 'B', and after an additional short time has moved to the position shown in 'C'. The magnitude of the y component of the bulk magnetization vector, M_y, as a function of time in the rotating frame (i.e. the FID), is plotted below (below, right). The decay in amplitude due to relaxation is ignored.

A   B   C

M_x

M_y

0   0.001   0.002   0.003
seconds
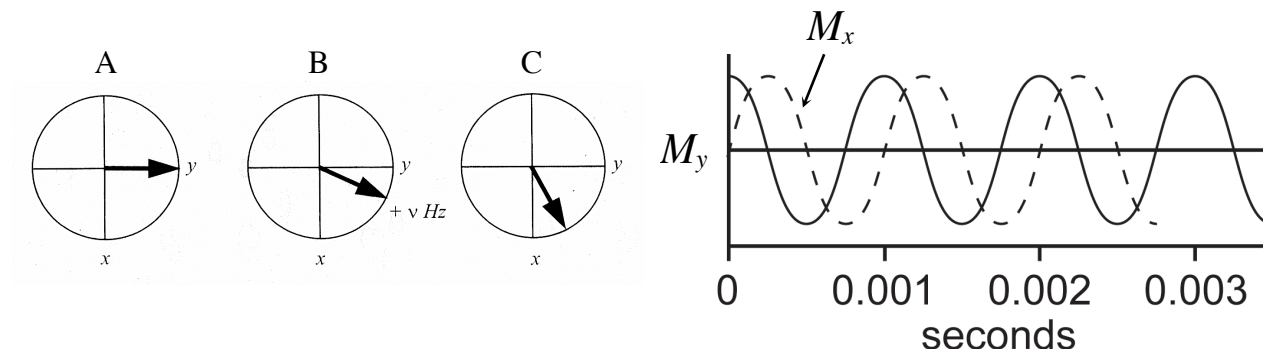
a. What is the frequency in the rotating frame for this ^1H nucleus? You must do a calculation and get an answer for credit. (**4 points**)

Each period, Δt, is 0.001 seconds, so:

$$v\,(or\,\Delta v) = 1/\Delta t = 1/0.001\;s = 1000\;Hz$$

b. The rotating frame frequency for a nucleus is determined from other frequencies. Please state what these are and exactly how the rotating frequency is calculated? (**4 points**)

The frequency in the rotating frame is the difference between the reference/carrier frequency (the frequency about which the high-power radio frequency pulse is applied) and the Larmor frequency, v_L, of the nucleus.

c. The figure (above, right) shows the magnitude of M_y for this nucleus plotted as a function of time. On the same graph, plot M_x for this nucleus versus time. (**4 points**)

M_x is plotted (dashed line) versus time. In 'A' (immediately after the pulse, at t = 0), the magnitude of the x component of the magnetization vector, M_x, is 0. As the bulk magnetization vector moves with time, first to its position in 'B' and then 'C', the magnitude of the x component of the magnetization vector increases. When the vector is aligned along the x axis, M_x is at its maximum. When plotted with M_y, the two waves are shown to be 90º out of phase with one another.

4). Shown (right) is the time-domain ^{1}H NMR data acquired for a particular compound that has only a single ^{1}H nucleus (for instance, $CHCl_3$).

0   1   2   3   4   5
seconds
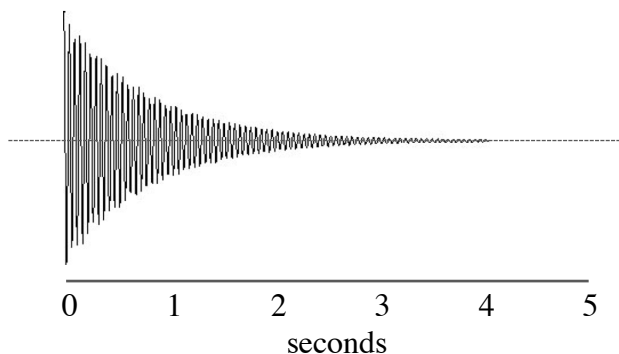
a. Estimate T_2 for this ^{1}H nucleus. For credit, you must do a calculation, get an answer, and your rationale must be clear. You must clearly describe any assumptions or approximations you make. (**6 points**)

The equation that governs the simple, first order loss of transverse magnetization by T_2 processes is:

$$M_y = M_0 e^{-t/T_2}$$

When ½ of the initial magnetization is lost (when M_y = ½ M_0), we have:

$$\frac{1}{2}M_0 = M_0 e^{-t/T_2} \quad \frac{1}{2} = e^{-t/T_2} \quad \ln\left(\frac{1}{2}\right) = -t/T_2 \quad T_2 = -\frac{t}{\ln\left(\frac{1}{2}\right)} = -\frac{t}{-0.693} = \frac{t}{0.693}$$

So, to __estimate__ T_2, estimate the time it takes for ½ of the initial magnetization to be lost (signal amplitude is about ½ of its maximum value). For the data shown, this is perhaps about ~1 second. Then use that to calculate the estimated T_2:

$$T_2 = \frac{t}{0.693} = \frac{1\,s}{0.693} = 1.44\,s \cong 1.4\,s$$

b. What is T_1 for this ^{1}H nucleus? Please explain for credit. (**6 points**)

It isn't possible to determine T_1 from the data shown. However, because $T_1 \geq T_2$, from the estimate of T_2 from part 'a', we can estimate a lower limit to T_1 (1.4 s).

5). For a sample containing a molecule with a single ^{1}H nucleus (i.e. CHCl$_3$), you are given a finite, limited amount of time to acquire a one-dimensional ^{1}H NMR spectrum of the sample.

$$d_1 \qquad AQ$$
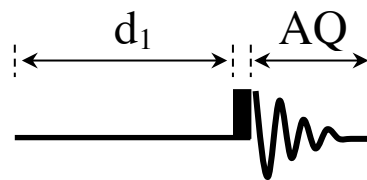
a. You have only about 1 minute to acquire data, and you decide to set d$_1$ to 1 second. What should the pulse angle be to give maximum signal-to-noise. Assume the acquisition time (AQ) is 2 s, the T$_1$ for the ^{1}H nucleus is 5 s, and the width of the pulse is only a few microseconds. (**4 points**)

For a given, finite, limited amount of time, the highest signal-to-noise is generated using the Ernst angle as the pulse angle. In this case, with the given values for the acquisition time (2 s) and T$_1$ (5 s), with d$_1$ = 1 s, the Ernst angle is calculated to be ~57°:

$$\cos \alpha_{Ernst} = e^{-((d_1+AQ)/T_1)} \qquad \alpha_{Ernst} = \cos^{-1}[e^{-((d_1+AQ)/T_1)}] \qquad \alpha_{Ernst} = \cos^{-1}[e^{-((1+2)/5)}] = 56.7°$$

b. Typical ^{1}H NMR spectra are acquired with acquisition times (AQ) on the order of 3T_2*, which usually allows for nearly complete decay of transverse relaxation between scans. Also, for typical small and medium sized organic molecules, $T_1 \approx T_2$, and for well-shimmed magnets, T_2* $\approx$ T_2. Given these facts, what can you say about the magnitude of the optimal pulse angle for most typical ^{1}H NMR spectra for typical organic molecules? (**4 points**)

The above facts, therefore, argue that typical acquisition times are 3T_1. Thus, d$_1$+AQ is at least 3T_1. According to Ernst, therefore,

$$\cos \alpha_{Ernst} = e^{-((d_1+AQ)/T_1)} \qquad \alpha_{Ernst} = \cos^{-1}[e^{-((d_1+AQ)/T_1)}] \qquad \alpha_{Ernst} > \cos^{-1}[e^{-(3)}] = 87°$$

This suggests that the optimal pulse angle for most of these types of experiments is nearly 90°.

6). Explain why, for an ensemble of spin ½ nuclei at thermal equilibrium, there is a net, bulk, macroscopic magnetization vector (M_0) along the *z*-axis, and in the +*z* direction, but there is no net macroscopic magnetization along either the *x*-axis, the *y*-axis, or anywhere in the *x-y* plane. (**8 points**)

> *At thermal equilibrium, for an ensemble of spin ½ nuclei, the individual nuclear magnetic dipoles are oriented either with (α states) or against (β states) the main magnetic field (B_0). The B_0 field is oriented in the +z direction. Because the dipoles in the a state are oriented with the B_0 field (+z direction), they are lower in energy, and, therefore, there are more of these than dipoles in the β state. The macroscopic M_0 vector is obtained by summing the individual magnetic dipoles of all of the nuclei. Because the number of α states is larger than the number of β states, the net result of summing the z-components (projections of the individual dipole vectors on the z-axis) is a bulk, macroscopic magnetic vector in the +z direction. There is no net component in the x-y plane because the individual dipole vectors are randomly arranged about the z-axis. So, the sum of x and y projections in any direction in the x-y plane is zero.*

7). The thermodynamics of T_1 and T_2^* processes are much different. One of these process is purely entropic and the other is purely enthalpic. Please explain which is which and why. (**8 points**)

If we define entropy simply as 'disorder', then the process of T_2^* would appear to be a purely entropic process. At thermal equilibrium, the individual magnetic dipole vectors are <u>randomly</u> distributed around the z-axis. This is a relatively disordered state. Application of the pulse creates <u>order</u> in the form of phase coherence among the vectors. As a function of time, entropy (disorder) increases, as it must, and the phase coherence is lost as the system returns to the more disordered equilibrium state.

Recall that the net result of applying a pulse is absorption of energy (net change of lower energy α states to higher energy β states). In order for the sample to return to thermal equilibrium, the energy/heat has to be taken out of the sample. This is accomplished by interactions of the spins with all components of the lattice, and, eventually, the energy is transferred to the walls of the sample tube and then to the outside of the sample tube where a stream of air carries away the excess heat (T_1 relaxation). Thus, transfer of energy via the lattice components leads ultimately to thermal equilibrium. This of course is an enthalpic process, essentially removing energy as heat following a pulse. So, T_1 relaxation is enthalpic.

8). For an electromagnetic pulse applied for 10 μs (at the Larmor frequency for a particular ^1H nucleus), the pulse angle is 90 degrees ($\pi/2$ radians). Calculate the strength (in Tesla) of this pulse? (**6 points**)

*We know that the pulse angle (Θ, in radians) is related to the gyromagnetic ratio (γ), the pulse length (τ_p) and the applied electromagnetic field strength (**B_1**) as shown:*

$$\Theta = \gamma B_1 \tau_p$$

Thus,

$$B_1 = \frac{\Theta}{\gamma \tau_p} = \frac{\pi/2 \ \text{rad}}{26.7519 \times 10^7 \ \text{rad T}^{-1}\text{s}^{-1} \ \times \ 10 \times 10^{-6}\text{s}} = 0.000587 \ \text{T}$$

9). Define "Larmor frequency" as it applies to NMR. Use complete sentences and no symbols, equations or drawings. (**4 points**)

In a static magnetic field, the angular momentum of a spin/nucleus orients itself with the field. The associated magnetic moment or nuclear dipole is also oriented at a specific angle with respect to the static field. The dipole rotates about the static field with an axis of rotation parallel to the field. In analogy to a spinning top, this motion is referred to as precession. The frequency of precession – the angular velocity or speed (radians/sec) of precession – for a given nucleus is referred to as its Larmor frequency.

10). You record an ^{13}C NMR spectrum of your compound using 1000 scans. You realize that you need to improve the sensitivity (signal-to-noise) by 4-fold. How many scans will be required to record a spectrum with 4 times the signal-to-noise? **(4 points)**

> *Signal-to-noise (S/N) increases as the square root of the number of scans ($S/N \propto N^{1/2}$). In order to improve S/N by 4×, one would have to acquire 4^2 or 16× the number of scans. So, if 1000 scans were used initially, 16×1000=16000 scans would be required for a 4× S/N improvement.*

$$\frac{1}{\sqrt{1000}} = \frac{4}{\sqrt{x}} \qquad \sqrt{x} = 4 \times \sqrt{1000} = 126.49 \qquad x = 126.49^2 = 16000$$

11). For nuclei that possess a magnetic moment, discrete energy levels (Zeeman levels/states) are occupied in the presence of a magnetic field.

a. What is the value of the spin angular momentum quantum number, **I**, for a particular nucleus that has six Zeeman levels? For full credit you will have to explain your reasoning. **(4 points)**

> *The number of possible Zeeman energy levels is equal to (2I+1), where 'I' represents the spin angular momentum quantum number. If (2I+1) = 6, then I = 5/2.*

b. If the magnetic quantum number, **m**, for one of the Zeeman energy levels for a particular nucleus is -2, what is the energy of this Zeeman energy level. **(2 points)**

> *In general, the energy, E, is described by the following equation:*

$$E = -m\gamma\hbar B_0$$

> *If m = -2, then:*

$$E = 2\gamma\hbar B_0$$

c. If the magnetic quantum number, **m**, for one of the Zeeman energy levels for a particular nucleus is -2, what is the spin angular momentum quantum number for this nucleus? Please explain. **(4 points)**
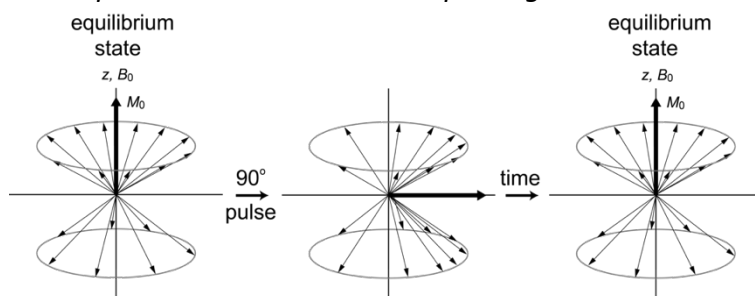
> *For a given nucleus, possible values of m are I, I-1, I-2,......-I. Thus, if m = -2, the spin quantum number must be integral (not half-integral), and must be $\geq$ 2.*

12). A simple pulse sequence for collecting a 1D NMR spectrum is shown (right). Following a delay (d_1), a 90° pulse is applied along the *x*-axis. After the pulse, the data are acquired for a time (indicated by the decaying sinusoidal line) and stored in the computer. The data consist of amplitude of the acquired signal as a function of time. As a function of time following the pulse, the amplitude of the signal decays until it reaches zero amplitude, or nearly zero (what's left is noise).
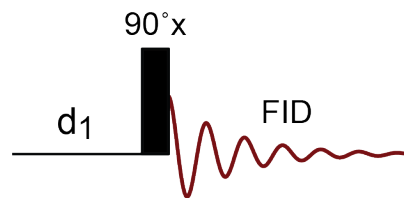
a). In the course notes, it states that the oscillating signal decays as a function of time, "as the phase coherence between the precessing magnetic dipoles (vectors) is lost". Please explain what is meant by the time-dependent loss of phase coherence between the precessing magnetic dipoles. (**6 points**)
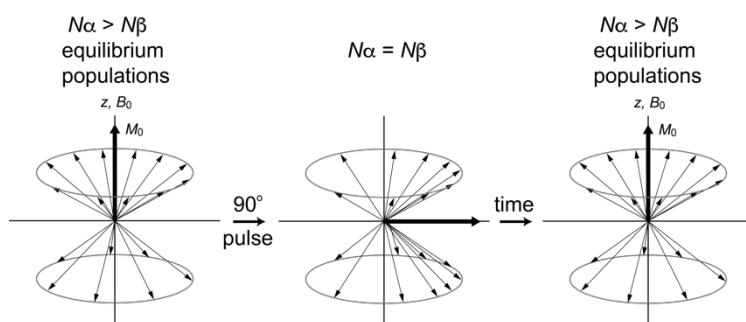
Following the pulse, the individual dipole vectors are bunched up along one axis in the transverse plane. They are no longer randomly dispersed about the z-axis. This is phase coherence. The dipole vectors precess together, but slowly, over time, they once again become randomly dispersed about the z-axis. Thus, the phase coherence is lost with time. This is inherently obvious. After the perturbation of the dipoles by the pulse, we know inherently that the system must return to equilibrium after some amount of time

b). Following the pulse, what else changes (besides the distribution of the vectors about the *z*-axis? Then, what happens as a function of time? (**6 points**)

Before the pulse, at thermal equilibrium, the α and β state populations are at their equilibrium values, with $N\alpha > N\beta$. Following the pulse, these populations are perturbed from their equilibrium values. If the pulse is a 90° pulse $N\alpha = N\beta$. As a function of time following the pulse, these populations will slowly return to their equilibrium values. We know inherently that this must be true. The pulse perturbs the equilibrium populations, but these populations must return to their equilibrium values with time.

13). If we directly compare ^1H spins and ^2H spins:

a. Calculate the ratio of the bulk/macroscopic magnetization ($M_{0\ 1H}/M_{0\ 2H}$) produced for equal numbers of ^1H and ^2H nuclei? **(6 points)**

$$\frac{M_{0\ 1H}}{M_{0\ 2H}} = \frac{\dfrac{N\gamma_{1H}^2\hbar^2 B_0 I_{1H}(I_{1H}+1)}{3k_BT}}{\dfrac{N\gamma_{2H}^2\hbar^2 B_0 I_{2H}(I_{2H}+1)}{3k_BT}} = \frac{\gamma_{1H}^2 \times \frac{1}{2}\left(\frac{1}{2}+1\right)}{\gamma_{2H}^2 \times 1(1+1)} = \frac{(26.7519\times 10^7\ \text{rad/Ts})^2 \times \frac{3}{4}}{(4.1066\times 10^7\ \text{rad/Ts})^2 \times 2} = 15.91$$

So, the bulk magnetization is about 16 times as large for ^1H as for ^2H.

b. Calculate how the sensitivities of the NMR signals compare for ^1H and ^2H spins? **(6 points)**

Sensitivity is proportional to the electromotive force (ε) induced in the receiver coil by the bulk magnetic moment. The magnitude of ε is proportional to the rate of change in the magnetic moment ($\varepsilon \propto dM/dt = \gamma M_0 B$).

Remember, $M_0 = \dfrac{N\gamma^2\hbar^2 B_0 I(I+1)}{3k_BT}$, *so* $\varepsilon \propto \gamma M_0 B = \dfrac{N\gamma^3\hbar^2 B_0^2 I(I+1)}{3k_BT}$. *Thus, whereas the magnitude of the bulk magnetization was dependent on γ^2, the sensitivity is dependent on γ^3.*

$$\frac{\varepsilon_{1H}}{\varepsilon_{2H}} = \frac{\dfrac{N\gamma_{1H}^3\hbar^2 B_0^2 I_{1H}(I_{1H}+1)}{3k_BT}}{\dfrac{N\gamma_{2H}^3\hbar^2 B_0^2 I_{2H}(I_{2H}+1)}{3k_BT}} = \frac{\gamma_{1H}^3 I_{1H}(I_{1H}+1)}{\gamma_{2H}^3 I_{2H}(I_{2H}+1)} = \frac{(26.7519\times 10^7\ \text{rad/Ts})^3 \times \frac{3}{4}}{(4.1066\times 10^7\ \text{rad/Ts})^3 \times 2} = 103.7$$

So, ^1H nuclei are about 104 times more sensitive than ^2H nuclei.

c. Fill in the blank: ^2H, ^{10}B, ^{11}B, ^{25}Mg, and ^{133}Cs are collectively referred to as __quadrupolar__ nuclei by NMR spectroscopists. **(2 points)**

For NMR spectroscopists, if the spin quantum number, I, for a nucleus is ≥ 1, then the nucleus is called a quadrupolar nucleus.

14). For a sample of $CHCl_3$, you apply a very long (seconds), low power pulse at the ^1H frequency of the single ^1H nucleus in the molecule. Immediately after this pulse, you apply a normal, high power 90° pulse at the same frequency and then record the FID. Sketch what you would expect the FID to look like. Also, sketch the spectrum you would expect to observe following Fourier transformation of the FID. You must thoroughly explain your answers for credit. (**6 points**).

A long pulse leads to equilibration of the α and β spin populations of the nucleus. In such an instance, there is no net, bulk (macroscopic) magnetization in either the longitudinal direction or transverse plane. If some longitudinal component were present, the 90 degree pulse would rotate that component into the transverse plane and it could then be detected. Because there is no such component, the 90 degree pulse does nothing, and there is no detectible signal. So, the FID will just be noise, and there will be no observable signals in the transformed spectrum.

15). You acquired a ^1H NMR spectrum of your sample. The spectral width (SW) was 6000.00 Hz. The acquisition time (AQ) was 2.0 seconds.

a. When the FID was digitized, how many points were collected/sampled? (**4 points**)

We know the relationship between the acquisition time (AQ, in seconds), the number of points (NP) and the sweep width (SW, in Hz):

$$AQ = NP/(2 \times SW)$$

Thus, NP=AQ$\times$2$\times$SW=2$\times$2$\times$6000=24,000

b. If more points had been sampled, would the digital resolution improve or worsen. You will have to explain your answer for credit. (**4 points**)

The digital resolution (DR, in Hz/pt), is defined as follows:

$$DR=1/AQ=2 \times SW/NP$$

Smaller values of DR indicate improved digital resolution. Thus, if more points had been samples (if NP increases), then DR gets smaller (digital resolution improves).

16). In NMR, for an experiment using a single pulse (i.e. a 'one scan' experiment), the maximum signal-to-noise is obtained if the pulse is a 90° pulse.

a. Explain why a 90° pulse gives the maximum signal-to-noise for a one scan experiment. (**6 points**)

> *In NMR, the signal-to-noise is dependent on the projection of M_0 in the x-y plane. The larger the projection, the higher the signal-to-noise (the larger the initial amplitude of the FID). A 90° pulse moves the entire M_0 vector into the x-y plane, by definition. Therefore, the highest signal-to-noise is obtained with a 90° pulse.*

b. Explain why it is often advantages to use shorter pulses (i.e., pulses shorter than 90°) if the amount of time available to perform an NMR experiment is limited. (**6 points**)

> *Using 90° pulses, the recovery time (time between pulses, approximately d1+AQ) must be very long to allow the magnetization to return to equilibrium (allow the populations of Na and Nb to return to their values at thermal equilibrium). This takes about $5 \times T_1$, so, for experiments where lots of scans are required, this can be an unexceptably long time. Using shorter pulses (pulse angles less than 90°), the signal generated from each pulse is less, but data from many more scans can be collected in the same amount of time. The tradeoff usually favors shorter pulses, and this can be calculated according to the Ernst angle equation (see part 'c').*

Name _____

THIS PAGE IS BLANK. FEEL FREE TO USE IT AS "SCRATCH" IF YOU LIKE

You may find some of the information below useful:

Table 1-1.
Properties of some nuclides of importance in NMR spectroscopy.

Nuclide	Spin I	Electric quadrupole moment[a] $[eQ]$ $[10^{-28}\ m^2]$	Natural abundance) [%]	Relative sensitivity[b]	Gyromagnetic ratio γ[a] $[10^7\ rad\ T^{-1}\ s^{-1}]$	NMR frequency [MHz][b] ($B_0 = 2.3488\ T$)
^1H	1/2	–	99.985	1.00	26.7519	100.0
^2H	1	2.87×10^{-3}	0.015	9.65×10^3	4.1066	15.351
^3H[c]	1/2	–	–	1.21	28.5350	106.664
^6Li	1	-6.4×10^{-4}	7.42	8.5×10^{-3}	3.9371	14.716
^{10}B	3	8.5×10^{-2}	19.58	1.99×10^{-2}	2.8747	10.746
^{11}B	3/2	4.1×10^{-2}	80.42	0.17	8.5847	32.084
^{12}C	0	–	98.9	–	–	–
^{13}C	1/2	–	1.108	1.59×10^{-2}	6.7283	25.144
^{14}N	1	1.67×10^{-2}	99.63	1.01×10^{-3}	1.9338	7.224
^{15}N	1/2	–	0.37	1.04×10^{-3}	–2.7126	10.133
^{16}O	0	–	99.96	–	–	–
^{17}O	5/2	-2.6×10^{-2}	0.037	2.91×10^{-2}	–3.6280	13.557
^{19}F	1/2	–	100	0.83	25.1815	94.077
^{23}Na	3/2	0.1	100	9.25×10^{-2}	7.0704	26.451
^{25}Mg	5/2	0.22	10.13	2.67×10^{-3}	–1.6389	6.1195
^{29}Si	1/2	–	4.70	7.84×10^{-3}	–5.3190	19.865
^{31}P	1/2	–	100	6.63×10^{-2}	10.8394	40.481
^{39}K	3/2	5.5×10^{-2}	93.1	5.08×10^{-4}	1.2499	4.667
^{43}Ca	7/2	-5.0×10^{-2}	0.145	6.40×10^{-3}	–1.8028	6.728
^{57}Fe	1/2	–	2.19	3.37×10^{-5}	0.8687	3.231
^{59}Co	7/2	0.42	100	0.28	6.3015	23.614
^{119}Sn	1/2	–	8.58	5.18×10^{-2}	–10.0318	37.272
^{133}Cs	7/2	-3.0×10^{-3}	100	4.74×10^{-2}	3.5339	13.117
^{195}Pt	1/2	–	33.8	9.94×10^{-3}	5.8383	21.499

B_0 (Tesla, T)	Resonance frequencies (MHz)	
	^1H	^{13}C
9.4	400	100.6
11.74	500	125.7
14.09	600	150.9
18.79	800	201.2

$\gamma_{1H} = 26.7519 \times 10^7\ rad/T/s, I = 1/2$

$\gamma_{10B} = 2.8747 \times 10^7\ rad/T/s, I = 3$

$\gamma_{11B} = 8.5847 \times 10^7\ rad/T/s, I = 3/2$

$\gamma_{13C} = 6.7283 \times 10^7\ rad/T/s, I = 1/2$

$\gamma_{15N} = -2.7126 \times 10^7\ rad/T/s, I = 1/2$

$\gamma_{17O} = -3.6280 \times 10^7\ rad/T/s, I = 5/2$

You may find some of the following information or equations useful:

$k_B = 1.381 \times 10^{-23}$ J/K
Avagadro's number $= 6.02214179 \times 10^{23}$ mol^{-1}

$h = 6.626 \times 10^{-34}$ Js
$\hbar = h/(2\pi)$

$P = \hbar\sqrt{I(I+1)}$
$P_Z = m\hbar$

$\mu = \gamma P = \hbar\gamma\sqrt{I(I+1)}$
for $m = \frac{1}{2}, \cos(\theta) = \frac{m\hbar}{\hbar\sqrt{I(I+1)}} = \frac{m}{\sqrt{I(I+1)}}$

$\pi/2$ radians $= 90°$

$$M_0 = \frac{N\gamma^2\hbar^2 B_0 I(I+1)}{3k_B T}$$

$$B_2 = \frac{\Delta\nu\sqrt{J^2-J_r^2}}{Jr} = \frac{J\Delta\nu}{Jr}$$

$$\varepsilon \propto dM/dt = \gamma M_0 B = \frac{N\gamma^3\hbar^2 B_0^2 I(I+1)}{3k_B T}$$

$$\Delta\nu = \nu_{BS} - \nu_0 = \frac{B_2^2}{2(\Delta B)} = \frac{B_2^2}{2(\nu_0-\nu_i)}$$

$S/N \propto NS^{1/2}$ (signal-to-noise improves with (number of scans)$^{1/2}$)

$m = (-I, -I+1, -I+2,\ldots., I)$ $(2I+1)$

$E = -\mu_Z B_0 = -m\gamma\hbar B_0$

$\Delta E = \mu_Z B_0 = \gamma\hbar B_0 = h\nu_L = h\nu_1$

$\nu_L = |\gamma/(2\pi)| B_0 = \omega_0/(2\pi)$

$\omega_0 = \gamma B_0$

$\Delta\delta = \dfrac{\Delta\nu}{\text{observe frequency}} \times 10^6$

$M_y = M_0 e^{-t/T_2^*}$
$M_z = M_0(1 - e^{-t/T_1})$
$M_z = M_0(1 - 2e^{-t/T_1})$

$\Delta\upsilon_{1/2} = \dfrac{1}{\pi T_2 *}$

$\dfrac{1}{T_2 *} = \dfrac{\gamma\Delta B_0}{2} + \dfrac{1}{T_2}$ $\dfrac{1}{T_2^*} = \dfrac{1}{T_2} + \dfrac{1}{T_2(B_0)}$

$t_{zero} = T_1\ln(2)$
$\eta = \gamma_a / (2\gamma_x)$
$I = (1 + \eta) I_0$
$I \propto 1/r^6$

$\Theta = \gamma B_1 \tau_p$

$\dfrac{N_\beta}{N_\alpha} \approx 1 - \left(\dfrac{\gamma\hbar B_0}{k_B T}\right)$

$B_{eff} = B_0(1-\sigma)$

$\upsilon_L = \dfrac{\gamma}{2\pi}(1-\sigma)B_0$

SW=1/(2DW)=Nyquist frequency (ν_{NQ})/2
AQ=DW*TD
DR=2SW/TD=1/AQ
(TD≡NP)

$\cos\alpha_{Ernst} = e^{-((d_1 + AQ)/T_1)}$
$\pi/2$ radians $= 90°$

$1+ \gamma_A/\gamma_X$ $1-\gamma_A/\gamma_X$

multiplicity$=2nI + 1$
$\Theta=2\pi J\tau$