

NMR FACILITY
User's Guide

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I. Introduction

The NMR Facility consists of ten superconducting magnet systems. One system is dedicated to solid state operation, four of the systems are proton/carbon switchable for routine organic applications. All of the spectrometers are LUNIX based systems running either Varian's VnmrJ software or Bruker's TopSpin software under the RedHat operating system.

There are three full time staff positions in the facility, providing service spectra, help planning and interpreting experiments, repair and maintenance of the equipment, hardware and software modification for special experiments, and instruction for users.

Researchers making extensive use of NMR in their research are encouraged to become checked out on the equipment so that they can obtain their own data. Instruments are available to authorized users 24 hours a day, 7 days a week.

II. Experiments Available

A wide variety of experiments may be performed on high-resolution solution state NMR spectrometers. One dimensional techniques are generally concerned with either the chemical shifts or the intensities of NMR signals, either as a probe to molecular structure or as a measure of some form of chemical dynamics. Two dimensional techniques are generally used to further resolve one dimensional spectra by spreading them out into a second frequency dimension and thereby simplifying them.

A. One Dimensional NMR

One dimensional NMR normally refers to those spectra or experiments that collect one or only a few FIDs or data sets. These spectra are treated as separate entities rather than as a matrix or two dimensional array. These experiments can array up to 18 different values for one of the acquisition parameters, permitting collection of data as a function of that parameter. Normally arrayed parameters include a D2 period for relaxation time studies, temperature for coalescence studies, and pre-acquisition delay for time kinetics.

1. 'Normal' spectra

Routine proton and carbon spectra typically consist of a single data set and provide chemical shift and intensity information. System software can provide lists of frequencies and intensities, as well as integrations, baseline corrections and other normal data processing functions.

2. Heteronuclear Spectra

Heteronuclear NMR normally refers to observing nuclei other than proton and carbon. Heteronuclear NMR can be complicated by a variety of factors including low natural abundance, low resonant frequency, quadrupole moments, and either very long or very short relaxation times. Very often, the information gained from heteronuclear spectra is in the form of coupling patterns to adjacent magnetically active nuclei, rather than from the chemical shift itself. Frequently, compounds with a heteroatom have only one heteronucleus to observe, so that integrated intensities and chemical shift differences are of much less importance. A single heteroatom in a sensitive area of large molecule can provide an effective probe into the molecule however.

Appendices I and II contain tabulations of resonant frequencies for all magnetically active nuclei, along with several other important numbers. The spin quantum number is used to calculate coupling patterns, and indicates the number of energy levels available to the nuclear spin. Spin 1/2 nuclei are generally the best behaved spectroscopically, especially since they cannot have an electric quadrupole moment. Nuclei with a spin greater than 1/2 can have a quadrupole moment, which will very often result in very rapid relaxation and broad lines, especially in asymmetric environments. ^{14}N with spin 1 has an electric quadrupole moment of only 0.07, but it broadens the ^{14}N resonances so completely that the only chemically useful information from nitrogen comes from the spin 1/2 ^{15}N species, even though it only has 0.37% natural abundance. This results in the need to enrich species in ^{15}N in order to observe them, and is the primary reason that nitrogen has not enjoyed greater popularity as a probe for NMR investigations.

3. Attached Proton Test

The Attached Proton Test (APT) spectrum provides information on the number of protons directly bound to a carbon. By using the coupling information to modulate the intensity of the carbon resonances, a spectrum is obtained in which the quaternary and methylene carbons are upright, and the methine and methyl carbons are inverted, providing useful information to help assign a carbon spectrum. This experiment depends on the scalar J coupling to modulate the signal intensity, and some peaks are consequently arbitrarily short or missing, so that it is necessary to run this spectrum in addition to a normal carbon spectrum, not instead of it. Normal practice is to plot the normal carbon and the APT spectrum on the same chart paper with the same scales for easy comparison.

In principle, the APT spectrum could be used with any heteronucleus exhibiting proton coupling. As noted above, however, heteronucleus spectra are generally simple enough that it is not worth the effort, especially since it depends on an accurate value for the coupling constant.

4. DEPT

DEPT (Distortionless Enhancement by Polarization Transfer) is a pulse sequence originally conceived to enhance nitrogen sensitivity by transferring polarization from protons to nitrogen. A specialized version is currently used to obtain information about the number of protons on a carbon. By changing the flip angle applied to the protons, the intensity of the carbon signal is modulated as a function of the number of attached protons, in a manner similar to that of the attached proton test, but by a different mechanism. By collecting four different spectra and taking linear combinations of them it is possible to generate edited subspectra, with separate traces showing only methyl, methylene, or methine carbons. Quaternary carbons are not observed by this technique since it requires a coupled proton spin for the polarization transfer. The advantage of this sequence is that the carbon multiplicities are assigned unambiguously. The disadvantage is that it requires four separate data acquisitions and consequently more time than the APT spectrum.

5. INEPT

INEPT (Insensitive Nuclei Enhancement by Polarization Transfer) is one of a variety of specialized pulse sequences that seek to enhance the sensitivity of low gamma nuclei by transferring polarization from a high gamma nucleus, usually protons. This permits observing the insensitive nucleus with sensitivity comparable to the higher gamma nucleus, and also permits repeating the experiment at a repetition rate determined by the high gamma nucleus T_1 which is usually shorter, at least for protons. The sequence depends on scalar J coupling to perform the polarization transfer, and thus requires *a priori* knowledge of the coupling constant. Nuclei that have no resolved J coupling cannot be observed by this technique. This tends to be more useful for very specialized determinations rather than for routine observation of low gamma nuclei. It is also useful for selectively exciting only those nuclei that are coupled to different nucleus. Thus, deuterium-carbon INEPT has been used to observe only carbons coupled to

deuterium, suppressing the carbon signals coupled to protons. Since deuterium has a lower gamma than does carbon, this also has the effect of lowering the sensitivity of the carbon experiment. While the INEPT sequence is no longer routinely used by itself, it is a fundamental unit of many two dimensional sequences.

6. Variable Temperature

The ability to control the temperature of the NMR sample provides the capability of performing a variety of different experiments. Heating samples to increase solubility and/or mobility, and cooling samples to stop or slow exchange processes are two examples. By determining the coalescence temperature for an exchange, it is also possible to determine the activation energy for the exchange.

7. Relaxation Times

Transverse and longitudinal relaxation times can be measured quite readily on any of the superconducting systems. The longitudinal relaxation time T_1 is the more commonly measured since it is the time that will determine the rate at which pulse experiments can be repeated. The transverse relaxation T_2 will determine linewidths and is generally of less interest. The mechanism for measuring either is the same. In the case of T_1 , a 180° pulse is used to invert the Z-axis magnetization. After a variable relaxation period the Z-axis magnetization is sampled with a 90° read pulse. A series of 6 to 10 spectra are run with different delay times, and then the Z-axis magnetization is plotted as a function of recovery time and fit to a first order exponential. The spectrometer computer system can automatically measure the various intensities, plot them, and do the iterative fitting to calculate the T_1 value. T_2 is measured the same way, except that initially a 90° pulse is used to create X-axis magnetization and one or more 180° echo pulses are used to remove chemical shift effects.

8. Time evolution kinetics

It is possible to collect a series of spectra as a function of time to watch the appearance of product peaks and/or the disappearance of reactant peaks in the spectrum. Peak intensities from these spectra can then be measured and fit to first order reaction kinetics. Other than first order kinetics requires processing on something besides the spectrometer computer system. Up to 18 different spectra can be collected, and they need not be evenly spaced in time, so that spectra can be collected more frequently at the beginning as the intensities change quickly, and less frequently later on as the intensities change more slowly.

9. Diffusion constants

On systems that include Pulsed Field Gradients, it is possible to run a series of spectra and measure diffusion constants for one or more species present in the sample or self-diffusion constants for neat liquids. This can be useful for estimating molecular sizes, distinguishing monomers from dimers, etc. The experiment consists of exciting the spins and allowing them to evolve in an inhomogeneous field. The spins are then refocused in the same inhomogeneous field. If there is no diffusion, the spins refocus perfectly and no signal intensity is lost. The more the spins diffuse during the echo period, the more the signal intensity is decreased. Calibration is normally done by comparing values obtained from a known standard such as water at 25 degrees.

B. Two Dimensional NMR

Two dimensional NMR provides the ability to spread a normal one dimensional spectrum out into a second frequency domain. In order to do this, a series of several hundred spectra are collected, varying a time period in the pulse sequence. These spectra are then rotated and fourier transformed a second time, with respect to the time scale defined in the pulse sequence, resulting in a two dimensional data table with two frequency axes. One axis will always be the chemical shift axis for the nucleus being observed. This is

the normal axis for the several hundred spectra that were collected. The second axis is determined by the pulse sequence used, and is usually either another chemical shift axis, or a J or coupling axis. The resolution of this second axis is determined by the number of spectra used to obtain the two-dimensional data set, and it is not necessarily limited by magnetic field inhomogeneities, but in some cases only by T_2 relaxation.

1. COSY

COSY (CORrelated SpectroscopY) is the first of the two dimensional experiments to be developed. It simply correlates homonuclear chemical shifts by J coupling. The second frequency axis is also a chemical shift axis, and the data table is normally square. The diagonal line with $\delta_1 = \delta_2$ is the normal one dimensional spectrum and off-diagonal or cross peaks at frequency coordinates δ_1, δ_2 indicate a scalar coupling between chemical shifts δ_1 and δ_2 . There will also be a comparable cross peak at δ_2, δ_1 .

There are now also a variety of 'new, improved' versions of the basic COSY experiment. PSCOSY is a phase sensitive version that gives sharper lines and therefore inherently better resolution. DQCOSY is a phase sensitive version that adds a double quantum filter to remove or suppress singlets on the main diagonal, making it easier to observe cross peaks near the diagonal ($\delta_1 \approx \delta_2$).

2. NOESY/ROESY

The NOESY (Nuclear Overhauser Effect SpectroscopY) is very similar in appearance to the COSY spectrum. The difference is that the cross peak generation is governed by dipole-dipole cross relaxation processes rather than scalar coupling. This is the same mechanism that gives rise to the NOE, and hence the name of the experiment. Dipole-dipole interactions tend to be more prevalent in high molecular weight molecules that tumble slowly in solution, so that this experiment tends to be more useful to protein chemists than to synthetic organic chemists working with relatively small molecules.

Related to this is the ROESY spectrum, the so called Rotating frame Overhauser Effect SpectroscopY, which uses a spin lock to permit nuclear Overhauser correlations on smaller molecules. This experiment requires linear power amplifiers and is currently possible only on the Unity, UnityPlus, and Inova spectrometers.

3. HETCOR

HETCOR (HETeronuclear CORrelated) is the heteronuclear version of the COSY experiment. The second frequency axis is a heteronuclear chemical shift, usually proton since the decoupler channel is used to generate the necessary frequencies. Cross peaks here indicate a scalar coupling between a proton chemical shift and a carbon (or phosphorus or nitrogen etc.) chemical shift. Since the two chemical shift axes are not the same, the data table is not necessarily nor usually square.

4. HMQC

HMQC is a variation of the HETCOR experiment, giving much the same kind of information, but getting the correlation information by means of a Heteronuclear Multiple Quantum Coherence, which comes about because of the scalar J coupling. The advantage of this experiment is that it observes through the proton spectrum, rather than the carbon, so that sensitivity is much greater. This does require being able to decouple the carbon spectrum during the observation period, which is not a trivial problem. The Inova-400, Unity+300, Unity500, Unity+500, and Inova-500 all have indirect detection probes and the signal switching necessary to support this type of experiment.

5. J-Resolved Spectra

The second frequency axis can also be a J axis rather than a chemical shift axis. The coupling can be either homonuclear proton-proton coupling (HOM2DJ) or heteronuclear proton-carbon or proton-phosphorus etc. (HET2DJ). In either case, a spectral slice through a given chemical shift gives the coupled resonance pattern without chemical shift information. Extraneous peaks arise in the homonuclear case if there is strong (non-first order) coupling present.

6. DOSY Spectra

DOSY (Diffusion Orded SpectroscopY) makes use of Pulsed Field Gradients to separate a one dimensional spectrum based on diffusion constants rather than other spectroscopic parameters. The indirectly detected dimension is diffusion constant rather than a frequency, so that in a mixture of several different compounds, the various compounds will generate separate spectra based on their size and diffusion. This provides a mechanism for obtaining separate spectra for the different components in a mixture without have to physically separate them using chromatographic techniques.

C. Solid-State Spectroscopy

NMR of samples in the solid state presents extra challenges compared to solution state spectroscopy. In solution, dipolar couplings and chemical shift anisotropies are averaged to zero. Dipolar interactions also cause faster T_2 relaxation so that resonances are significantly broader in solid state spectra. In order to make these samples observable, several different techniques are employed. High power dipolar decoupling is used to removed dipolar couplings, high speed sample spinning (3-5 Khz or more) at the so called magic angle ($54^\circ 44'$) is used to remove chemical shift anisotropy, and cross polarization techniques are used to improve sensitivity.

III. Equipment Available

The following paragraphs contain brief descriptions of the various instruments available in the NMR facility. An emphasis has been placed on detailing those features which differ between the various instruments and those features that are important for choosing an instrument for a given experiment, and not necessarily on details or differences that are internal to the instruments and not of direct concern to users.

A. Avance500

The Avance 500 is a 4 channel system with a cryoprobe. The cryoprobe cools the reciever coil and preamplifier electronics to $40-50^\circ$ K, reducing themal noise, increaing the coil Q and making dramatic improvements in sensitivity. Proton sensitivity is approximately 9 times that of a conventional probe, generating close to 2 orders of magnitude in time savings. This probe is a triple resonance probe that has a proton observe channel and Carbon and Nitogen decoupling channels. It is also possible to do direct observation through these decoupler coils, although the sensitivity improvements are not as great as those for proton observation. There is no other heteronuclear capability on this system, and the probe is much more fragile and susceptible to damage from improper parameters.

B. NMRS-500 RM

The NMRS-500 is a 500 Mhz system with 4 full RF channels and a $^1\text{H}/^{19}\text{F}/^{31}\text{P}/^{13}\text{C}$ quad nucleus probe and 4 separate preamplifiers. The probe is also rated for low temperatures, down to -150° C. This makes the system ideal for studying both exchanging systems and systems with complex heteronuclear

coupling. It is straightforward to do multinuclear decoupling experiments such as $^1\text{H}\{^{19}\text{F}\}\{^{31}\text{P}\}$ or even $^{13}\text{C}\{^1\text{H}\}\{^{19}\text{F}\}\{^{31}\text{P}\}$. The four preamplifiers eliminate the need for cable swapping as the system is configured for different observe nuclei.

C. Inova500B

The Inova500B (formerly the UnityPlus 500) is a 500 MHz superconducting system that has been customized for biological NMR studies on peptides and proteins. It has two completely broadband RF channels, a PFG (pulsed field gradient) accessory, deuterium gradient shimming capability, waveform generators for shaped pulses on both RF channels, variable temperature accessory, and a 39 channel high purity room temperature magnet shimming system. The magnet shimming system permits very high quality lineshapes to be obtained non-spinning, facilitating water suppression experiments. The primary probe on this system is a 5 mm indirect detection probe.

D. NMRS 500

The NMRS-500 (formerly the Unity500) is also a 500 MHz superconducting system that has been customized for biological NMR studies on peptides and proteins. It includes four broadband RF channels, all with pulse shaping and variable power for a variety of selective excitation experiments. The primary probe on the system is a 5 mm broadband probe. The system also includes triple resonance proton probe with carbon and nitrogen coils. The UNIX based software permits both 2 and 3 dimensional NMR studies. The Unity500 has several probes available for a variety of different experiments:

A 5mm broadband probe is available for direct observation of nuclei between ^{15}N and ^{31}P

A 5m triple resonance proton observe probe with carbon and nitrogen decoupling coils, for isotopically labeled protein $^1\text{H}\{^{13}\text{C}\}\{^{15}\text{N}\}$ 2 and 3D experiments.

A 3mm Carbon probe is available for direct observation of ^{13}C on samples where quantity is limited. The sample volume is approximately 100 μL , compared to 730 μL in the 5mm probe.

A 5mm Proton/Fluorine probe, capable of doing both $^1\text{H}\{^{19}\text{F}\}$ and $^{19}\text{F}\{^1\text{H}\}$ experiments.

E. Inova-500

The Inova-500 is a 500 MHz superconducting system that is equipped for a wide variety of high resolution experiments. It is configured as a proton/carbon system, with a switchable probe, two RF channels, variable temperature, and a Pulsed Field Gradient accessory.

F. Inova-400

The Inova-400 is a 400 MHz superconducting system that is equipped for a wide variety of high resolution experiments. It is a broadband RF system with a full set of 10 mm probes to observe heteronuclei from 160 MHz (^{31}P) down to 9 MHz (^{187}Os). It also has a 5 mm proton/fluorine probe, a 5 mm

$^1\text{H}\{\text{X}\}$ indirect detection probe, and a 5mm autoswitchable probe. The autoswitchable probe is normally installed on this system. It can be configured as either a 4-nucleus ($^1\text{H}/^{19}\text{F}/^{31}\text{P}/^{13}\text{C}$) probe or as a more conventional broadband probe ($^{15}\text{N}-^{31}\text{P}\{^1\text{H} \text{ or } ^{19}\text{F}\}$).

G. Avance-400

The Avance-400 is a Bruker spectrometer that provides solid state spectra. This is a Linux based spectrometer with a wide bore (89mm) actively shielded magnet dedicated to running solid state samples. Three CP-MAS probes (2.5, 4 and 7 mm) are available, with a maximum spinning rate of 30 KHz (2.5 mm probe). The system console has 3 fully broadband RF channels, permitting triple resonance experiments. The 4 mm probe is capable of HXY and FXY tuning, permitting 2D heteronuclear experiments with cross polarization from either proton or fluorine. This system also includes a static wideline probe with both 5 and 10 mm inserts. All probes are capable of variable temperature operation.

H. Inova-300

The Inova 300 (formerly the UnityPlus 300) spectrometer is an UNIX based spectrometer system operating at 300 MHz for proton spectra. This system is equipped with a Quad probe, capable of observing ^1H , ^{19}F , ^{31}P , and ^{13}C without any operator intervention. The console hardware includes a full broadband channel and a proton-only channel, permitting broadband proton decoupling on all heteronuclear spectra except ^{19}F . In addition, the system supports homonuclear proton decoupling and variable temperature operation. This system is capable of swapping the function of the observe and decouple channels so that it can perform the various indirect detection experiments such as HMQC and phosphorous decoupled proton spectra. It also has the attenuators and linear amplifiers necessary to perform spin lock experiments such as ROESY. The system has a 10 G/cm pulsed field gradient amplifier and deuterium gradient shimming accessory permitting both fast gradient shimming on deuterated solvents and gradient-enhanced 2 dimensional experiments.

I. Mercury Plus 300 Proton-Carbon

The Mercury Plus 300 is a routine access proton-carbon spectrometer operating at 300 MHz. It has a switchable probe with gradient coil, two RF channels, and a gradient amplifier for pulsed field gradient experiments. The ATB probe operates in a switchable mode, simultaneously tuned ^1H and ^{13}C , but the proton coil is double tuned to ^{19}F as well. This system is also capable of using pulsed field gradient to do deuterium gradient shimming.

J. NMRS-300

The NMRS-300 (formerly the VXR-300) spectrometer is also a UNIX-based system operating at 300 MHz for proton spectra. It has a broadband observation channel and a proton only decoupler channel and incorporates a proton/carbon switchable probe. This system provides routine ^1H and ^{13}C spectra and includes homonuclear proton decoupling capability. The NMRS-300 has a variable temperature controller, but does not normally provide variable temperature work since nitrogen gas is not available at the instrument. This instrument is part of the instrumentation for the Chemistry 233/234 organic majors lab, and is therefore unavailable for research use during class periods, especially during the spring semester.

IV. Off-line Data Processing

Three Dell Linux computers are available for performing off-line data processing of data from any of the superconducting magnet systems. Data can be transferred from any of the spectrometers (except for the Avance 400) to the workstations over ethernet and processed on the Dell computers using VnmrJ, Varian's workstation software that is identical to that on the NMRS, Inova, and Mercury spectrometers. This is an X-windows application which can be run remotely from any X-windows server, permitting remote processing of your spectral data. The workstations include HP LaserJet4 printers (8 1/2 by 11 inch plots) as output devices. CR_ROM drives and USB ports are available on all three workstations for archival storage of data.

Another Dell PC workstation is available, running the TopSpin software under Linux, providing an off-line processing and storage capability for the Avance 400 and Avance 500 spectrometers. This workstation is networked to the Sun workstations, permitting shared use of printer and plotter resources.

V. Access Procedure

There are full time staff spectroscopists available who will run service spectra on any of the instruments available in the facility. Spectral data can be archived to user-supplied media, and hardcopy output generated in any format useful to the end user. Due to limited instrument time and scheduling constraints, please allow at least several days for service work to be completed. Please contact one of the to discuss with the staff any special experiments or conditions that you may require and to arrange a time for your service work.

Any researcher within the chemistry department that wishes to be checked out on one or more of the spectrometers should register for an instruction class by filling out the web form at <http://www.chem.tamu.edu/nmr/forms>. Instruction on the routine access instruments is rapid (1-2 weeks) and only requires 2-3 hours to complete. This instruction is consequently very cursory and does not address many of the issues involved in getting good NMR data, nor does it include practice in the simpler procedures. Do not expect to get on the instruments with one or two days notice, and do not sign up for the course a year in advance. The instrument operation is complex enough, that if you do not begin using it on a regular basis after completing the course, you will forget everything you learned.

After a user has been checked out on the routine 1H/13C spectrometers, he can request access to the Inova-400, the variable temperature accessory on the Inova-300, and the walk-up Inova500 system. These are all considered more advanced functions and instruction is scheduled on an as-needed basis. The web registration form also has a link to a list of minimum expected skill necessary before advancing beyond the basic 300 Mhz instrumtents. Access to the Inova500b and NMRS-500 500 MHz systems as well the Avance 400 solids system is available for advanced users who need those capabilities. For limited amounts of work, service spectra can be obtained on any of these systems, but direct user access is the normal mode of operation.

A. Reservation System

Time may be reserved on all of the routine access instruments (Mercury 300, NMRS-300, Inova-300, Inova-400, Inova-500) using a computerized reservation system. This system gets a daily update from each of the spectrometers and knows the authorized users on each system, along with their instrument password. There is a separate rule base and reservation data base for each of the spectrometers, and any authorized user may log in to the system and make a reservation for instrument time. Anyone, whether a listed user or not, may log in to examine the reservation data base in order to determine whether time is

available on the system or to determine who has it reserved. In addition, there is a status screen for each of the systems, making it possible to learn of problems or scheduled down time without coming to the lab to read a note on the door. The following is a summary of the current reservation rules on the systems.

Mercury 300, Inova-300, NMRS-300, Inova-500: These instruments are all used for rapid access routine proton and carbon spectra and are reserved on same day-only basis. Reservation rules on the various systems differ, but generally users may reserve 30 minutes, in 10 minute blocks, between 8 AM and 10 PM, Monday through Saturday. 8 AM until 2 PM may be reserved after 8 AM, and 2 PM until 10 PM may be reserved after 1 PM. The overnight hours (10 PM to 8 AM) and Sunday may be reserved up to 3 days in advance, again in 10 minute blocks. There is no limit on the amount of overnight time that may be reserved. The NMRS-300 is in the undergraduate majors lab and is used for class instruction. Undergraduates using the system for class will generally have preferential reservation rules.

The Inova-400 instrument may be reserved up to 3 days in advance with no time restrictions.

The most current and complete summary of reservation rules is available on the NMR web site.

B. Instrument Status

Instrument status information is available on the instrument reservation system. As you log on to reserve time on an instrument system, an instrument status screen will be displayed automatically if the status information has changed within the past 3 days. Instrument status information may always be obtained using the S(tatus) command within the reservation system.

VI. Charges

Current hourly rates for using the NMR facilities are as follows:

Chemistry Department:

500 Mhz Cryoprobe system	\$12.25
500 MHz	\$9.25
400 MHz	\$7.25
300 MHz	\$5.25

Chemistry Department charges are capped at \$540/month maximum charge.

Other Departments on TAMU campus	\$15.00
Other Texas Universities	\$25.00
Other outside samples	\$75.00

VII. Appendix I, NMR Frequencies by Frequency

Nuclide	Spin	% Natural Abundance	Frequency on		Electric Quadrupole
			XL-200	Inova-400	
H - 3	1/2	.00	215.897	431.671	--
H - 1	1/2	99.98	200.053	399.992	--
F - 19	1/2	100.00	188.205	376.304	--
He- 3	1/2	.00	152.396	304.706	--
Tl-205	1/2	70.48	115.446	230.827	--
Tl-203	1/2	29.52	114.329	228.591	--
P - 31	1/2	100.00	80.983	161.921	--
Li- 7	3/2	92.57	77.746	155.449	.10
Sn-119	1/2	8.68	74.565	149.089	--
Sn-117	1/2	7.67	71.273	142.505	--
Rb- 87	3/2	27.20	65.458	130.877	.14
Sn-115	1/2	.35	65.415	130.793	--
B - 11	3/2	81.17	64.185	128.333	.04
Te-125	1/2	7.03	63.199	126.361	--
Ga- 71	3/2	39.80	61.009	121.981	.11
Pr-141	5/2	100.00	58.733	117.434	.05
Cu- 65	3/2	30.91	56.804	113.574	.15
Xe-129	1/2	26.24	55.338	110.646	--
Br- 81	3/2	49.43	54.027	108.022	.28
Cu- 63	3/2	69.09	53.026	106.022	.16
Na- 23	3/2	100.00	52.918	105.806	.10
V - 51	7/2	100.00	52.579	105.130	.20
Te-123	1/2	.89	52.438	104.846	--
Al- 27	5/2	100.00	52.128	104.226	.15
C - 13	1/2	1.11	50.300	100.570	--
Br- 79	3/2	50.57	50.121	100.214	.34
Eu-151	5/2	47.77	49.613	99.198	.00
Mn- 55	5/2	100.00	49.342	98.654	.60
Nb- 93	9/2	100.00	48.899	97.770	.16
Sc- 45	7/2	100.00	48.597	97.166	.22
Ga- 69	3/2	60.20	48.021	96.014	.18
Sb-121	5/2	57.25	47.875	95.722	.53
Co- 59	7/2	100.00	47.239	94.450	.50
Tb-159	3/2	100.00	45.391	90.754	.00
Re-185	5/2	37.07	45.039	90.054	2.80
Cd-113	1/2	12.34	44.380	88.734	--
In-113	9/2	4.16	43.746	87.466	.75
Pt-195	1/2	33.70	42.780	85.534	--
Cd-111	1/2	12.86	42.418	84.810	--
Pb-207	1/2	21.11	41.857	83.690	--
Ho-165	7/2	100.00	41.020	82.018	2.00
I -127	5/2	100.00	40.026	80.030	.75
Si- 29	1/2	4.70	39.740	79.458	--
Se- 77	1/2	7.50	38.145	76.266	--
Hg-199	1/2	16.86	35.653	71.287	--

NMR Frequencies by Frequency

Nuclide	Spin	% Natural Abundance	Frequency on		Electric Quadrupole
			XL-200	Inova-400	
Yb-171	1/2	14.27	35.235	70.451	--
As- 75	3/2	100.00	34.264	68.507	.30
H - 2	1	.02	30.711	61.403	.00
Li- 6	1	7.43	29.441	58.867	.00
La-139	7/2	99.91	28.261	56.507	.50
Be- 9	3/2	100.00	28.113	56.211	.02
O - 17	5/2	.04	27.122	54.227	.00
Cs-133	7/2	100.00	26.242	52.471	.00
Sb-123	7/2	42.75	25.925	51.835	.68
Ta-181	7/2	100.00	23.943	47.871	4.00
Lu-175	7/2	97.40	22.836	45.659	5.70
Ba-137	3/2	11.32	22.230	44.447	.00
Eu-153	5/2	52.23	21.911	43.811	.00
B - 10	3	18.83	21.498	42.983	.07
N - 15	1/2	.37	20.271	40.531	--
V - 50	6	.24	19.946	39.879	.00
Ba-135	3/2	6.59	19.874	39.735	.00
Cl- 35	3/2	75.40	19.599	39.187	.08
Rb- 85	5/2	72.80	19.315	38.619	.28
Zr- 91	5/2	11.23	18.664	37.319	.00
Ni- 61	3/2	1.25	17.877	35.743	.00
Tm-169	1/2	100.00	16.539	33.067	--
Xe-131	3/2	21.23	16.405	32.799	.12
Cl- 37	3/2	24.60	16.315	32.619	.06
Ne- 21	3/2	.26	15.792	31.575	.00
Os-189	3/2	16.10	15.523	31.035	2.00
S - 33	3/2	.74	15.344	30.679	.05
N - 14	1	99.64	14.451	28.895	.07
Ca- 43	7/2	.13	13.458	26.907	.00
Mo- 97	5/2	9.60	13.309	26.611	.00
Hg-201	3/2	13.24	13.123	26.239	.45
Mo- 95	5/2	15.78	13.033	26.059	.00
Zn- 67	5/2	4.12	12.512	25.015	.18
Mg- 25	5/2	10.05	12.241	24.475	.00
Cr- 53	3/2	9.54	11.307	22.608	.00
Ti- 49	7/2	5.51	11.277	22.548	.00
Ti- 47	5/2	7.75	11.277	22.548	.00
Nd-143	7/2	12.20	10.877	21.748	.57
Se- 79	7/2	.00	10.430	20.856	.70
Ru-101	5/2	16.98	9.869	19.732	.00
Y - 89	1/2	100.00	9.803	19.600	--
Yb-173	5/2	16.08	9.708	19.412	.00
Dy-163	5/2	24.97	9.399	18.792	.00
Gd-157	3/2	15.64	9.399	18.792	1.00
K - 39	3/2	93.08	9.336	18.668	.07

NMR Frequencies by Frequency

Nuclide	Spin	% Natural Abundance	Frequency on		Electric Quadrupole
			XL-200	Inova-400	
Ag-109	1/2	48.65	9.308	18.612	--
Pd-105	5/2	22.23	9.162	18.320	.00
Sr- 87	9/2	7.02	8.669	17.332	.00
W -183	1/2	14.28	8.325	16.644	--
Sm-147	7/2	15.07	8.270	16.536	.72
Ag-107	1/2	51.35	8.098	16.192	--
Kr- 83	9/2	11.55	7.696	15.388	.15
Gd-155	3/2	14.68	7.517	15.032	1.10
Ge- 73	9/2	7.61	6.977	13.952	.20
Ru- 99	5/2	12.81	6.768	13.532	.00
Nd-145	7/2	8.30	6.672	13.340	.30
Dy-161	5/2	18.73	6.577	13.152	.00
Sm-149	7/2	13.84	6.577	13.152	.72
Fe- 57	1/2	2.25	6.464	12.924	--
Rh-103	1/2	100.00	6.298	12.592	--
Hf-177	7/2	18.39	6.106	12.208	3.00
Er-167	7/2	22.82	5.779	11.556	.00
K - 41	3/2	6.91	5.123	10.244	.00
Os-187	1/2	.00	4.607	9.212	--
Hf-179	9/2	13.78	3.757	7.512	3.00
Ir-193	3/2	61.50	3.742	7.484	1.50
Ir-191	3/2	38.50	3.438	6.876	1.50
Au-197	3/2	100.00	3.425	6.848	.56

VIII. Appendix II, NMR Frequencies by Isotopic Mass

Nuclide	Spin	% Natural Abundance	Frequency on		Electric Quadrupole
			XL-200	Inova-400	
H - 1	1/2	99.98	200.053	399.992	--
H - 2	1	.02	30.711	61.403	.00
H - 3	1/2	.00	215.897	431.671	--
He- 3	1/2	.00	152.396	304.706	--
Li- 6	1	7.43	29.441	58.867	.00
Li- 7	3/2	92.57	77.746	155.449	.10
Be- 9	3/2	100.00	28.113	56.211	.02
B - 10	3	18.83	21.498	42.983	.07
B - 11	3/2	81.17	64.185	128.333	.04
C - 13	1/2	1.11	50.300	100.570	--
N - 14	1	99.64	14.451	28.895	.07
N - 15	1/2	.37	20.271	40.531	--
O - 17	5/2	.04	27.122	54.227	.00
F - 19	1/2	100.00	188.205	376.304	--
Ne- 21	3/2	.26	15.792	31.575	.00
Na- 23	3/2	100.00	52.918	105.806	.10
Mg- 25	5/2	10.05	12.241	24.475	.00
Al- 27	5/2	100.00	52.128	104.226	.15
Si- 29	1/2	4.70	39.740	79.458	--
P - 31	1/2	100.00	80.983	161.921	--
S - 33	3/2	.74	15.344	30.679	.05
Cl- 35	3/2	75.40	19.599	39.187	.08
Cl- 37	3/2	24.60	16.315	32.619	.06
K - 39	3/2	93.08	9.336	18.668	.07
K - 41	3/2	6.91	5.123	10.244	.00
Ca- 43	7/2	.13	13.458	26.907	.00
Sc- 45	7/2	100.00	48.597	97.166	.22
Ti- 47	5/2	7.75	11.277	22.548	.00
Ti- 49	7/2	5.51	11.277	22.548	.00
V - 50	6	.24	19.946	39.879	.00
V - 51	7/2	100.00	52.579	105.130	.20
Cr- 53	3/2	9.54	11.307	22.608	.00
Mn- 55	5/2	100.00	49.342	98.654	.60
Fe- 57	1/2	2.25	6.464	12.924	--
Co- 59	7/2	100.00	47.239	94.450	.50
Ni- 61	3/2	1.25	17.877	35.743	.00
Cu- 63	3/2	69.09	53.026	106.022	.16
Cu- 65	3/2	30.91	56.804	113.574	.15
Zn- 67	5/2	4.12	12.512	25.015	.18
Ga- 69	3/2	60.20	48.021	96.014	.18
Ga- 71	3/2	39.80	61.009	121.981	.11
Ge- 73	9/2	7.61	6.977	13.952	.20
As- 75	3/2	100.00	34.264	68.507	.30
Se- 77	1/2	7.50	38.145	76.266	--
Br- 79	3/2	50.57	50.121	100.214	.34

NMR Frequencies by Isotopic Mass

Nuclide	Spin	% Natural Abundance	Frequency on		Electric Quadrupole
			XL-200	Inova-400	
Se- 79	7/2	.00	10.430	20.856	.70
Br- 81	3/2	49.43	54.027	108.022	.28
Kr- 83	9/2	11.55	7.696	15.388	.15
Rb- 85	5/2	72.80	19.315	38.619	.28
Rb- 87	3/2	27.20	65.458	130.877	.14
Sr- 87	9/2	7.02	8.669	17.332	.00
Y - 89	1/2	100.00	9.803	19.600	--
Zr- 91	5/2	11.23	18.664	37.319	.00
Nb- 93	9/2	100.00	48.899	97.770	.16
Mo- 95	5/2	15.78	13.033	26.059	.00
Mo- 97	5/2	9.60	13.309	26.611	.00
Ru- 99	5/2	12.81	6.768	13.532	.00
Ru-101	5/2	16.98	9.869	19.732	.00
Rh-103	1/2	100.00	6.298	12.592	--
Pd-105	5/2	22.23	9.162	18.320	.00
Ag-107	1/2	51.35	8.098	16.192	--
Ag-109	1/2	48.65	9.308	18.612	--
Cd-111	1/2	12.86	42.418	84.810	--
Cd-113	1/2	12.34	44.380	88.734	--
In-113	9/2	4.16	43.746	87.466	.75
Sn-115	1/2	.35	65.415	130.793	--
Sn-117	1/2	7.67	71.273	142.505	--
Sn-119	1/2	8.68	74.565	149.089	--
Sb-121	5/2	57.25	47.875	95.722	.53
Te-123	1/2	.89	52.438	104.846	--
Sb-123	7/2	42.75	25.925	51.835	.68
Te-125	1/2	7.03	63.199	126.361	--
I -127	5/2	100.00	40.026	80.030	.75
Xe-129	1/2	26.24	55.338	110.646	--
Xe-131	3/2	21.23	16.405	32.799	.12
Cs-133	7/2	100.00	26.242	52.471	.00
Ba-135	3/2	6.59	19.874	39.735	.00
Ba-137	3/2	11.32	22.230	44.447	.00
La-139	7/2	99.91	28.261	56.507	.50
Pr-141	5/2	100.00	58.733	117.434	.05
Nd-143	7/2	12.20	10.877	21.748	.57
Nd-145	7/2	8.30	6.672	13.340	.30
Sm-147	7/2	15.07	8.270	16.536	.72
Sm-149	7/2	13.84	6.577	13.152	.72
Eu-151	5/2	47.77	49.613	99.198	.00
Eu-153	5/2	52.23	21.911	43.811	.00
Gd-155	3/2	14.68	7.517	15.032	1.10
Gd-157	3/2	15.64	9.399	18.792	1.00
Tb-159	3/2	100.00	45.391	90.754	.00
Dy-161	5/2	18.73	6.577	13.152	.00

NMR Frequencies by Isotopic Mass

Nuclide	Spin	% Natural Abundance	Frequency on		Electric Quadrupole
			XL-200	Inova-400	
Dy-163	5/2	24.97	9.399	18.792	.00
Ho-165	7/2	100.00	41.020	82.018	2.00
Er-167	7/2	22.82	5.779	11.556	.00
Tm-169	1/2	100.00	16.539	33.067	--
Yb-171	1/2	14.27	35.235	70.451	--
Yb-173	5/2	16.08	9.708	19.412	.00
Lu-175	7/2	97.40	22.836	45.659	5.70
Hf-177	7/2	18.39	6.106	12.208	3.00
Hf-179	9/2	13.78	3.757	7.512	3.00
Ta-181	7/2	100.00	23.943	47.871	4.00
W -183	1/2	14.28	8.325	16.644	--
Re-185	5/2	37.07	45.039	90.054	2.80
Os-187	1/2	.00	4.607	9.212	--
Os-189	3/2	16.10	15.523	31.035	2.00
Ir-191	3/2	38.50	3.438	6.876	1.50
Ir-193	3/2	61.50	3.742	7.484	1.50
Pt-195	1/2	33.70	42.780	85.534	--
Au-197	3/2	100.00	3.425	6.848	.56
Hg-199	1/2	16.86	35.653	71.287	--
Hg-201	3/2	13.24	13.123	26.239	.45
Tl-203	1/2	29.52	114.329	228.591	--
Tl-205	1/2	70.48	115.446	230.827	--
Pb-207	1/2	21.11	41.857	83.690	--