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FORTHCOMING NMR MEETINGS

Symposium on *In Vivo* Magnetic Resonance Spectroscopy VII, Monterey, California, April 9 - 10, 1994; Contact: Radiology Postgraduate Education; Room C-324, University of California School of Medicine, San Francisco, CA 94143-0628; Phone: (415) 476-5731; Fax: (415) 476-9213; For registration, call (415) 476-5808; Fax: (415) 476-0318.

35th ENC (Experimental NMR Conference), Asilomar Conference Center, Pacific Grove, California, April 10 - 15, 1994; Contact: ENC, 815 Don Gaspar, Santa Fe, NM 87501; (505) 989-4573; Fax: (505) 989-1073.

Gordon Conference on Order/Disorder in Solids, New London, New Hampshire, August 7 - 12, 1994; Contact: Prof. M. A. White, Dept. of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3; Tel. (902) 484-3894; Fax: (902) 494-1310. See TAMU NMR Newsletter 421, 44.

12th International Meeting on NMR Spectroscopy, Sponsored by the Royal Society of Chemistry, Manchester, England, July 2 - 7, 1995 [sic]; Contact: Dr. J. F. Gibson or Ms. G. B. Howlett - See TAMU NMR Newsletter 415, 5; Phone: (44-71) 437-8656; Fax: (44-71) 437-8883.

ISMAR 1995, Sydney, NSW, Australia, July 16-21, 1995 [sic]; Contact: Dr. Wm. A. Bubb, Secretary, Univ. of Sydney, Dept. of Biochemistry, Sydney, NSW 2006, Australia. See TAMU NMR Newsletter 419, 26.

Additional listings of meetings, etc., are invited.

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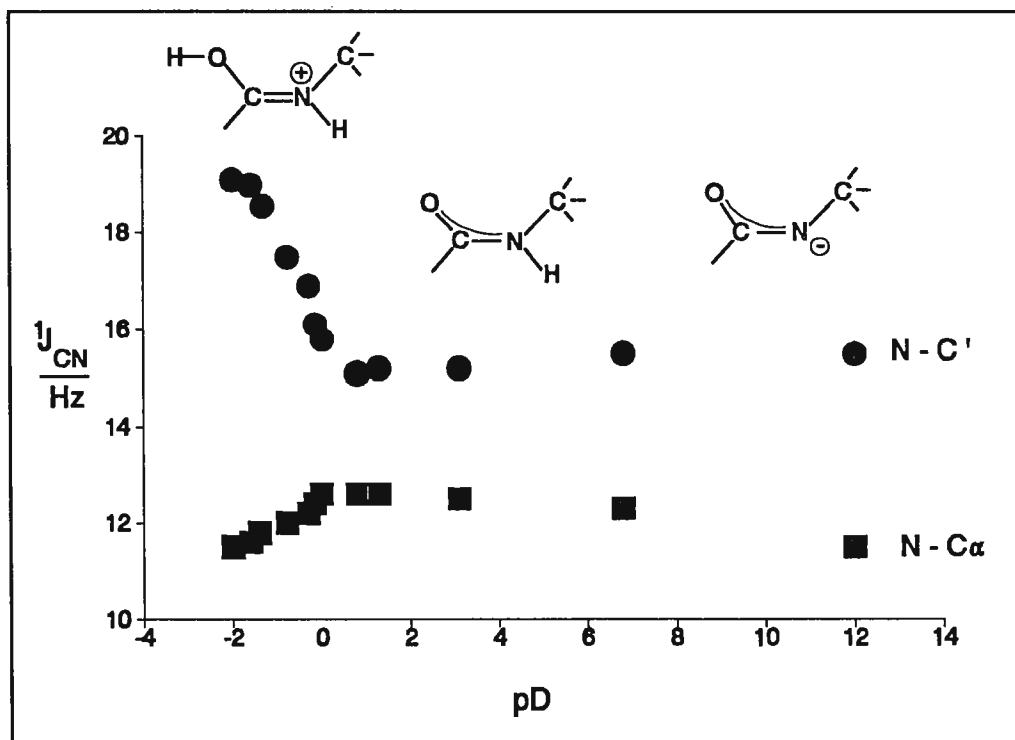
(received 8/26/93)
August 25, 1993

EFFECT OF HYDROGEN BONDING ON PEPTIDE BOND CARBON-NITROGEN COUPLINGS

Dear Professor Shapiro:

The use of ^{15}N - ^{13}C J couplings for obtaining information on peptides backbone conformation has been considered recently (F. Delaglio, D.A. Torchia, A. Bax, *J. Biomolecular NMR*, 1(1991)439). The results indicated that J_{NC} couplings are affected by protein backbone conformation. However, a possible correlation between the $^1J_{\text{NC}}$ couplings and the non-planarity of the peptide bond was not established.

The involvement of peptide bond moieties in the hydrogen bonding network of proteins may be one factor that obscures a simple correlation. An insight into the impact of hydrogen bonding on the $^1J_{\text{NC}}$ couplings we have afforded by investigation of pH dependence of the couplings in the double enriched (^{15}N , ^{13}C) N-acetyl-glycine (Figure).



Sincerely yours,

Nenad Juranic
Nenad Juranic
INTERNET:juranic@mayo.edu

S. Macura
Slobodan Macura
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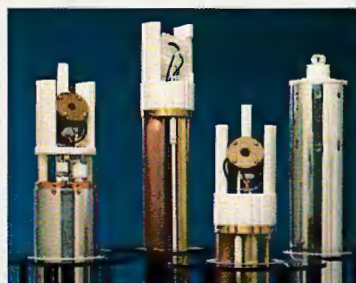
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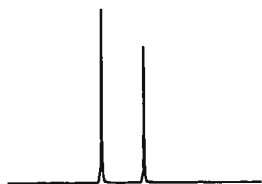
Variable Amplitude Cross Polarization - The Latest Technique from Chemagnetics

The introduction of the Variable Amplitude Cross Polarization (VACP) technique by Professor Steve Smith at the Yale University at the 1993 ENC may completely change the approach to optimization of solid state NMR experiments. This technique produces high quality solid state CP/MAS data, even on samples where the match condition may be impossible to optimize, such as weakly coupled systems. This opens up great potential for effective quantitation and comparison of data from different samples.

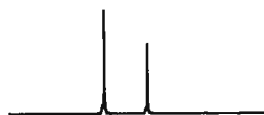
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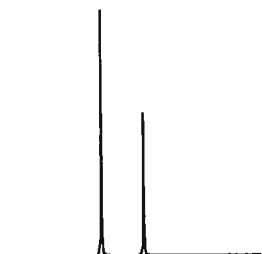
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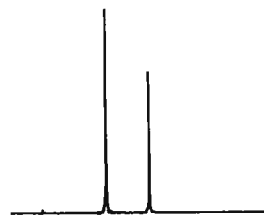
Variable amplitude cross polarization (VACP)
under -2.6 KHz mismatch condition



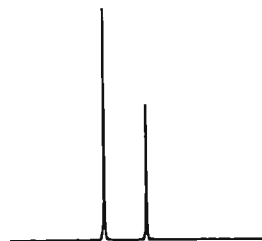
Deliberate "mismatch" of -1.9 KHz



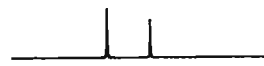
VACP under normal match condition



Normal "ideal" matched conditions



VACP under +2.0 KHz mismatch condition



Deliberate "mismatch" of +1.4 KHz

Chemagnetics would like to thank Professor Steve Smith for suggestion of this work and useful discussions during its implementation.



Cornell University

Biotechnology Program
130 Biotechnology Building
Ithaca, NY 14853-2703 USA
(607) 255-2300

Fax: (607) 255-2428
Email: Yang_Xia@qmrelay.mail.cornell.edu

September 12, 1993 (received 9/17/93)

Dr Bernard L. Shapiro
Editor,
Texas A&M NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

Please credit this communication to Dr. Aiden Harrison's account.

Displaying Images using Felix on a Silicon Graphics Workstation

Dear Barry,

Felix (formally Hare Research and now Biosym, San Diego CA) is a software package designed for multidimensional high-resolution spectroscopic analysis. The most powerful feature of Felix is its extensive macro program library and the facility of writing your own macros. We describe here how Felix can be used to display 2-D NMR images on a Silicon Graphics workstation. Four steps are involved in doing so: data transfer, data format translation, display program, and display parameters. The data format translation is a bit tricky and we are pleased to share it with your readers.

The first step is the data transfer. For those with spectrometers that are not equipped with an Ethernet, there was a recent communication in TAMU (415-29), which described a home-built hardware/software package that transfers data between the ASPECT 3000 and IBM PC. It turns out that Bruker (Billerica, MA) sells an inexpensive parallel communication package (NMR-Link) that can transfer data between the ASPECT 3000 and an IBM/Macintosh. Our imaging data are acquired using a Bruker AM spectrometer with an ASPECT 3000 computer, and transferred from the AM to a Macintosh Quadra via NMR-Link. The Mac is etherneted with a Silicon Graphics computer, where Felix is.

Once the data are on the SGI, some file format translation is required. There is a translation program, bris.f, which comes with Felix. We found that the byte-swap part of the program must be modified so that there is no swap of the first byte and the third byte (the data on the AM spectrometer are 24 bits long).

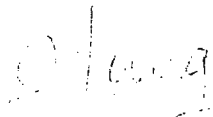
The next step is to write programs to process the data and display it. Our macro program consists of two parts: a main macro and a menu macro. The menu macro is used for setting up an input menu (see below). The main macro reads a 2-D serial file, performs a 2-D FT (either Bruker FT or FFT), and saves the final images as a mat file (a special matrix file used in Felix).

The image can then be displayed as an intensity plot in the 2-D mode of Felix. Note that the display parameters for the intensity plot must be set properly in order to display an image on the screen. We found that the Contour Level in Parameters must be set between 0.01 and 0.001 for displaying images.

Cross sectional profiles of the 2-D image can be exported as a text file, which can subsequently be processed using other commercial graph/fitting programs.

The macro programs are available from the authors upon request.

Best regards.


Yang Xia


Lynn W. Jelinski

Postdoctoral Position Available

There is an opening in my lab for a person to work on applications of solid state nmr to the study of materials. Requirements are a Ph.D. in Chemistry and some familiarity with solid state CPMAS NMR methods. Familiarity with Varian Sun-based (VXR/UNITY) instruments is also advantageous. Expected salary will be \$20,000/year. A one year appointment is available immediately, with renewal for a second year based upon availability of funds and mutual agreement. Three instruments are available for this work; a home-built 200 MHz solids instrument, a Unityplus-200 instrument dedicated to solids, and a Unityplus-600 with a supersonic MAS solids accessory. Between these instruments we have the capability to perform triple resonance solids experiments such as REDOR, variable temperature (-150° to + 250°), multinuclear experiments, and wide-line NMR. Interested applicants should have at least two letters of reference, cv, and copies of publications sent to: Prof. Peter Rinaldi, Department of Chemistry, The University of Akron, Akron, Ohio 44325-3601.

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The initial resurgence of interest in applying gradients to high resolution NMR spectroscopy focused on a single axis (z-gradient) probe design. Now, applications are being developed that require 3 gradients. GE NMR Instruments successfully pioneered three gradient high resolution probes with widely published results¹⁻⁴. A very important application is water suppression by diffusion weighting⁵. For example, figure 1 shows results in an improved phase-sensitive HMQC experiment in which diffusion filters are employed to avoid dynamic range problems⁶.

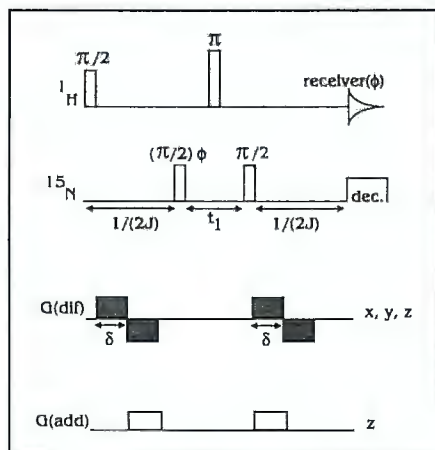


Figure 1a: Pulse sequence from reference 6

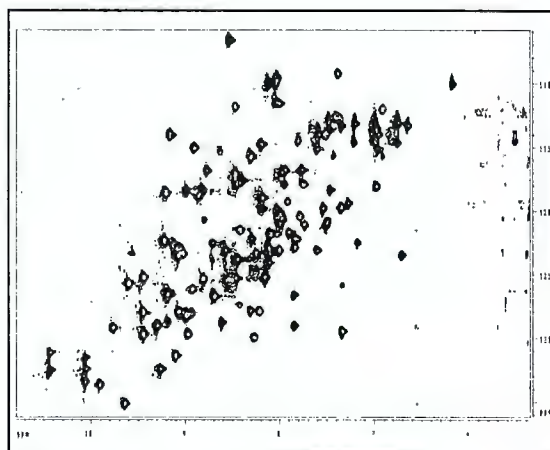
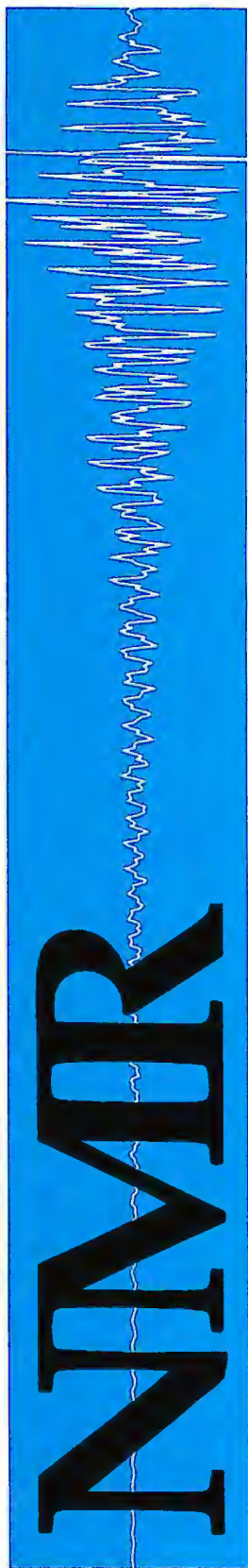


Figure 1b: 1.5mM of MutT in 90% H₂O/D₂O

With GRASP III, three gradient experiments are now available for all AVANCE users. Probes for 5mm samples are available in ¹H observe, inverse broadband, and triple resonance inverse configurations for 500, 600, and 750 MHz spectrometers. The compact ultra stable Acustar gradient amplifier enables z-gradient strength of up to 40 G/cm and x, & y-gradients of up to 35 G/cm! All of this packaged together with the excellent RF performance typical of Bruker probes.

NMR



Different orthogonal gradient directions can now be chosen for different functional uses of gradients such as "crusher" gradients, diffusion gradients, coherence selection gradients, slice selection gradients or gradients at the magic angle. The availability of three gradient axes greatly improves the capability to remove inadvertent and undesirable gradient-recalled echoes. The benefits are both greater ease-of-use as well as increased flexibility for new gradient spectroscopy pulse sequences.

The AVANCE is also revolutionizing gradient generation with its new Gradient Control Unit (GCU™). The GCU is interfaced to the VME bus and driven by a modern high performance embedded Intel i960 RISC processor.

Today, with increasing emphasis placed on gradients, the GCU is the logical hardware evolution from simple square gradient generation. The power of the i960 allows, for the first time, gradients to be calculated "on the fly" as dictated by the experimental requirements. The desired gradient is generated in real time by the microprocessor without the need for traditional memory for the gradient length or shape. Best of all, it can do this simultaneously for x, y, & z-gradients.

Up to now, NMR systems had to utilize dedicated memory to pre-define the desired gradients before the execution of the NMR experiment. In complex experiments, the memory size has lead to a limitation as the number of gradient pulses incorporated into a single sequence continued to grow. The GCU's revolutionary design overcomes this restriction. *In addition, the GCU can provide gradient shaping for all three gradients, on the fly!* The gradient shapes can be linear (to give trapezoidal shape), sinusoidal (for sine shape) or arbitrary functions.

GRASP III provides for traditional single gradient applications as well as for three gradient spectroscopy experiments. Together with the GCU, extreme versatility in creating novel experiments with shaped x, y, & z-gradients becomes reality!

reference:

1. R.E. Hurd, B.K. John, P. Webb, D. Plant. *J.Magn.Reson.* **99**, 632 (1992).
2. B.K. John, D. Plant, P. Webb, R.E. Hurd. *J.Magn.Reson.* **98**, 200 (1992).
3. R.E. Hurd. *J.Magn.Reson.* **87**, 442 (1990).
4. R.E. Hurd, D. Freeman. *Proc.Natl.Acad.Sci. USA.* **86**, 4402 (1989).
5. P.C.M. van Zijl, C.T.W. Moonen. *J.Magn.Reson.* **87**, 18-25 (1990).
6. P.C.M. van Zijl, M. O'Neil-Johnson, C. Abeygunawardana. *J.Magn.Reson.* (submitted).

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Wissembourg, September 14th 1993

(received 9/21/93)

Dear Barry,

B_0 pulse field gradients have proven to be very useful for NMR experiments involving a heteronucleus, the most impressive illustrations being reverse type experiments like the HMQC, HMBC or HSQC sequences¹.

However, when one wishes to use pulse field gradients solely for the purpose of water suppression in a simple NOESY experiment it becomes impossible to use gradient coherence selections to suppress the water, since the signals of interest and the water follow the same coherence pathway.

Recently, solutions have been proposed² to alleviate this problem. However the purpose of this communication is to show that the combination of gradients with the well known 1-1 echo³ sequence (Figure 1) can lead to a dramatic improvement of water suppression. This feature is due to the fact that the use of gradients in this sequence is equivalent to the 4 step Exorcycle⁴ phase cycle. This property insures very high water suppression per individual scan. Another advantage of the gradients in a NOESY sequence is that radiation damping becomes much less severe, allowing the use of very short mixing time.

A NOESY experiment using this technique was run on a DNA three way junction (TWJ)⁵ sample (2 mM in 90% H₂O) with three gradients of strength 21/31.5/31.5 G/cm and of duration 6ms/300 μ s/300 μ s. The spectrum shown in Figure 2 was obtained in 32 scans with a 150 ms mixing time and it shows that the quality of water suppression is almost perfect.

Sincerely,

M. PIOTTO

V. SKLENAR

N. LEONTIS

C. BREVARD

- ¹ A. Davis et al., *J. Magn. Reson.*, **98**, 207-216 (1992).
J.-M. Tyburn et al., *J. Magn. Reson.*, **97**, 305-312 (1992).
- ² M. Piotto et al., *J. Biomol. NMR*, **2**, 661-665 (1992).
- ³ V. Sklenar and A. Bax, *J. Magn. Reson.*, **74**, 469-479 (1987).
- ⁴ G. Bodenhausen et al., *J. Magn. Reson.*, **27**, 511 (1977).
- ⁵ N. Leontis et al., *in press*.

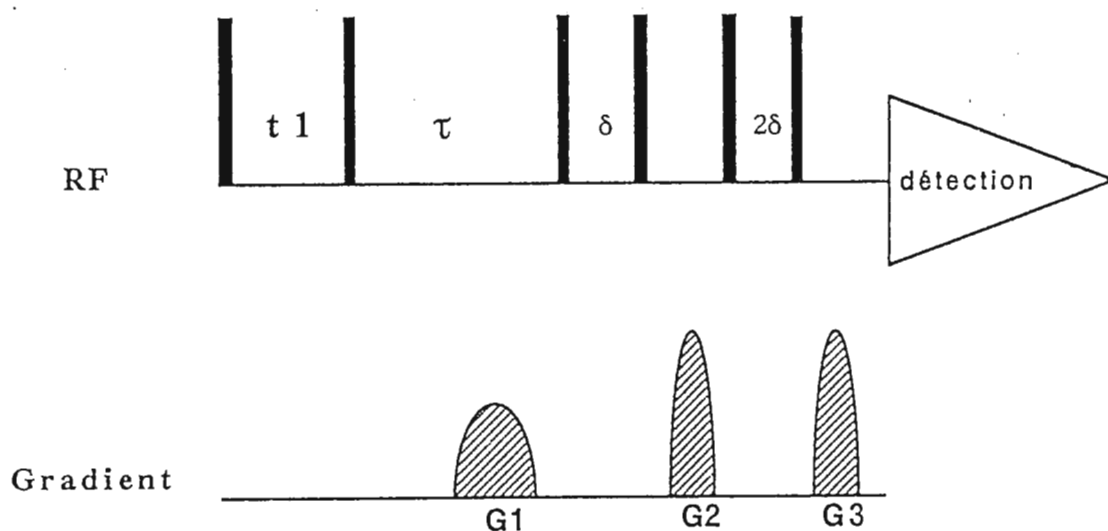


Figure 1: Pulse sequence of the NOESY 1-1 echo with gradients ($\delta=53\mu\text{s}$, $\tau=150\text{ ms}$, $G1=21\text{ G/cm}$, $G2=G3=31.5\text{G/cm}$).

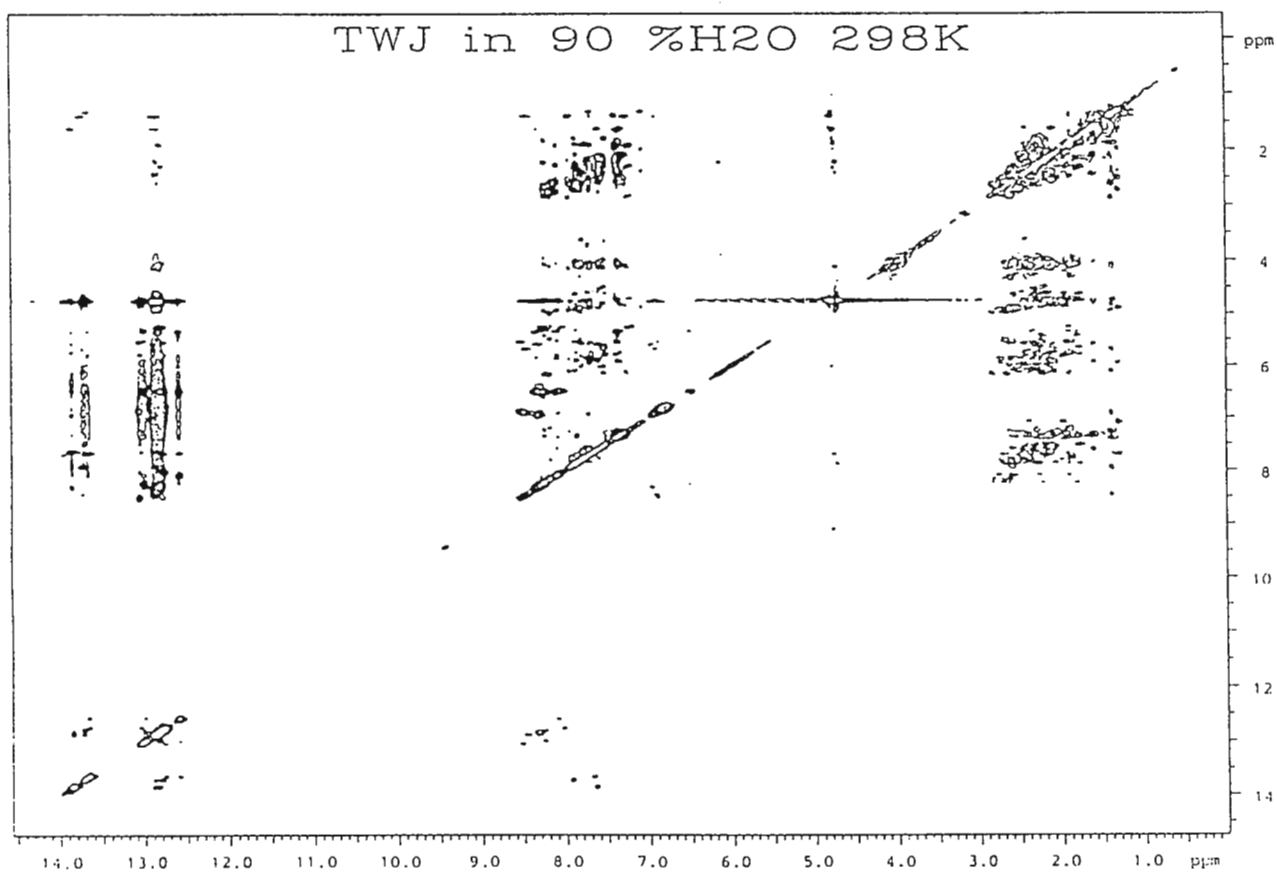


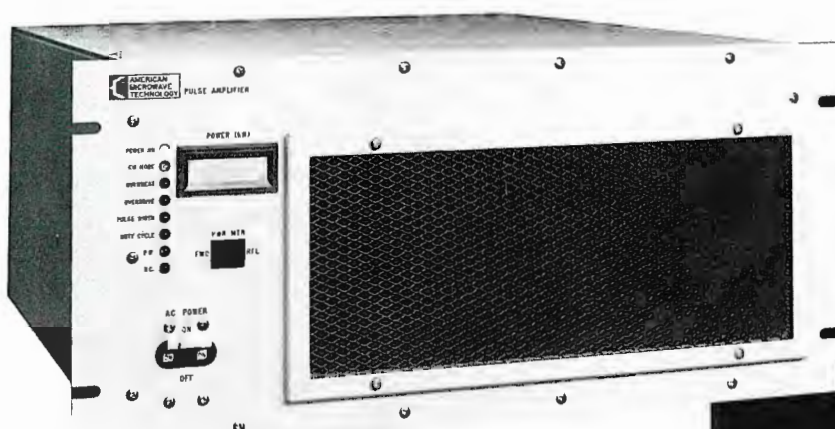
Figure 2: NOESY spectrum of a 32 base pair three way junction DNA sample in 90% H₂O.

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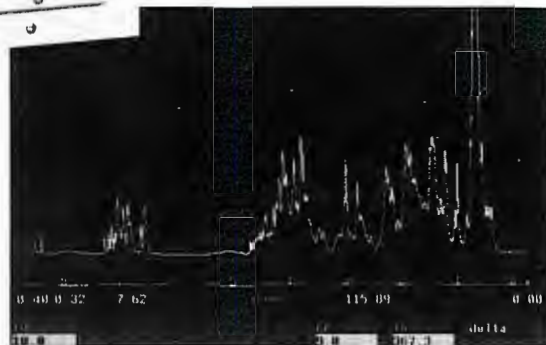
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- Linearity ± 1 dB
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3200	6–220 MHz	150 to 1000 W
3304	30–310 MHz	400 W
3420	10–90 MHz	1000 to 2000 W



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Electrical specifications:

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CW power (max.) into 50 ohms	100 W
Linearity (± 1 dB)	0–900 W
Gain (typ.)	65 dB
Gain flatness	± 2 dB
Input/Output impedance	50 ohms
Input VSWR	$< 2:1$
Pulse width	20 ms
Duty cycle	Up to 10%
Amplitude rise/fall time	250 ns typ.
Amplitude droop	5% to 20 ms typ.
Phase change/output power	10° to rated power, typ.
Phase error overpulse	4° to 20 ms duration, typ.
Noise figure	11 dB typ.
Output noise (blanked)	< 20 dB over thermal
Blanking delay	$< 2 \mu\text{s}$ on/off, TTL signal
Protection	1. VSWR: infinite VSWR 2. Input overdrive: up to 10 dB 3. Over duty cycle/pulse width 4. Over temperature

Supplemental characteristics:

Connectors, rear panel	1. RF input: BNC (F) 2. RF output: Type N (F) 3. Noise blanking: BNC (F) 4. Interface: 25 pin D(F), EMI filtered
Indicators, front panel	1. AC power on 2. Peak power meter 3. Over pulse width 4. Over duty cycle 5. Over temperature 6. Over drive 7. CW mode
System monitors	1. Forward/Reflected RF power 2. Over pulse width/duty cycle 3. DC power supply fault 4. Thermal fault
Front panel controls	1. AC power 2. Pulse width 3. Duty cycle
Cooling	Internal forced air
Operating temperature	$+10$ to 40°C
AC line voltage	208/230 VAC, $\pm 10\%$, 50–60 Hz
AC power requirements	2000 watts
Package	Rack mount
Size (HWD, inches)	$8.75 \times 19 \times 20.25$
Net weight	100 lbs.

03/92



Department of Chemistry
Buchtel College of Arts and Sciences
Akron, OH 44325-3601
216-972-7372

August 30, 1993
(received 9/17/93)

Dr. Bernard L. Shapiro, Editor
TAMU NMR Newsletter
966 Elsinore Ct.
Palo Alto, CA 94303

Subject: ^2H Lock and Decoupling, New Unityplus-600

Dear Barry,

After years of effort (mostly with fundraising) we are finally having fun solving problems with our new Varian Unityplus 600 MHz NMR. Among the new features which we had not anticipated is a lock circuit which is under software control through the standard pulse programming software.

We have been using this new instrument feature to perform experiments which require ^2H decoupling. In the past, we have performed these experiments on our older 300 MHz instrument in the unlocked mode. Field drift was minimal on this instrument, enabling us to acquire spectra overnight in unlocked mode without serious degradation of spectral resolution. Figure 1a is an example of a ^2H to ^{13}C INEPT spectrum of deuterated polybutadiene obtained with ^1H and ^2H decoupling during data acquisition.

The spectrum in Figure 1b is from an identical experiment which was performed on our 600 MHz spectrometer in an identical time. The lock was gated on for only the last 50 ms of a 500 ms relaxation delay. Despite the drift of the magnet, ability to control the lock channel during the pulse sequence enabled us to maintain a stable field over the course of the 4 hour experiment. The improved signal to noise in the 150 MHz spectrum arises from the higher sensitivity of the higher field instrument, partly from the higher quality Rf of the new generation instrument, and the absence of line broadening which results from field drift in the unlocked experiment.

Best Regards,

Lan Li
Research Assistant

Peter L. Rinaldi
Professor of Chemistry and Director
of Molecular Spectroscopy Laboratory

PBD#17-INEPT-3J
 PULSE SEQUENCE inept_dec2
 OBSERVE C13
 FREQUENCY 150.869 MHz
 SPECTRAL WIDTH 30007.5 Hz
 ACQUISITION TIME 0.400 sec
 RELAXATION DELAY 0.200 sec
 PULSE WIDTH 9.2 usec
 TEMPERATURE 30.0 deg. C.
 NO. REPETITIONS 20480
 DECOUPLE H1
 HIGH POWER 45
 DECOUPLER CONTINUOUSLY ON

 DOUBLE PRECISION ACQUISITION
 DATA PROCESSING
 LINE BROADENING 5.0 Hz
 FT SIZE 131072
 TOTAL ACQUISITION TIME 3.6 hours

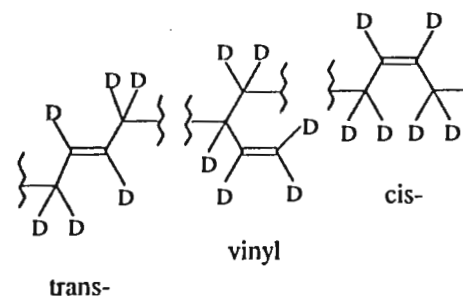
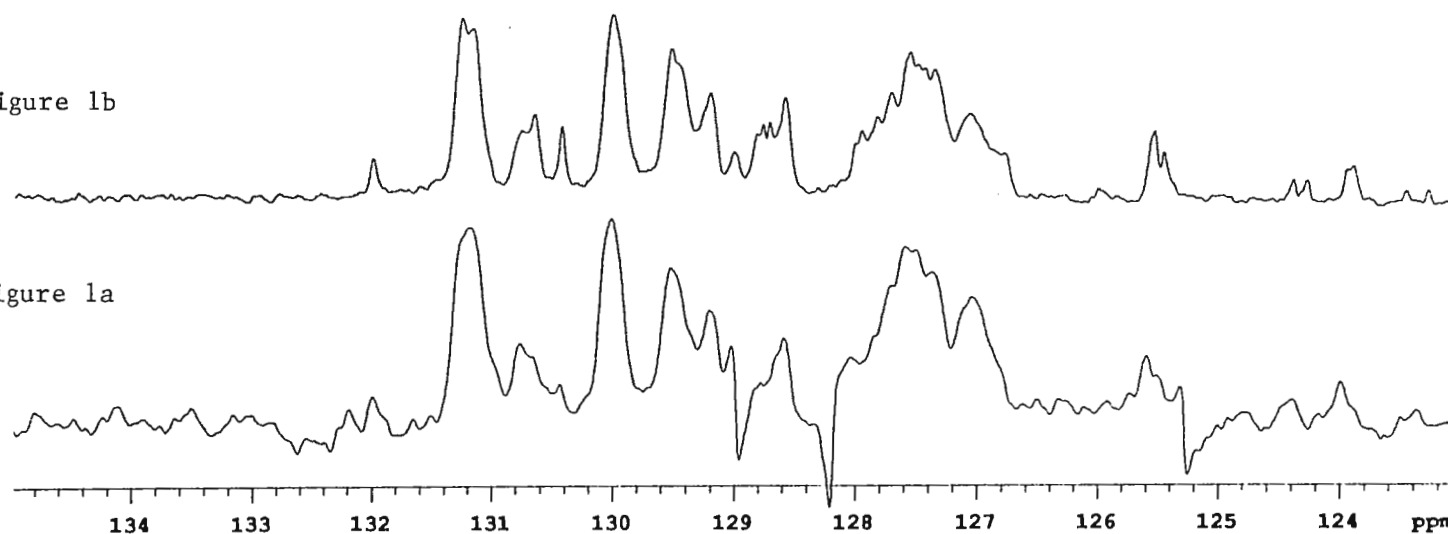
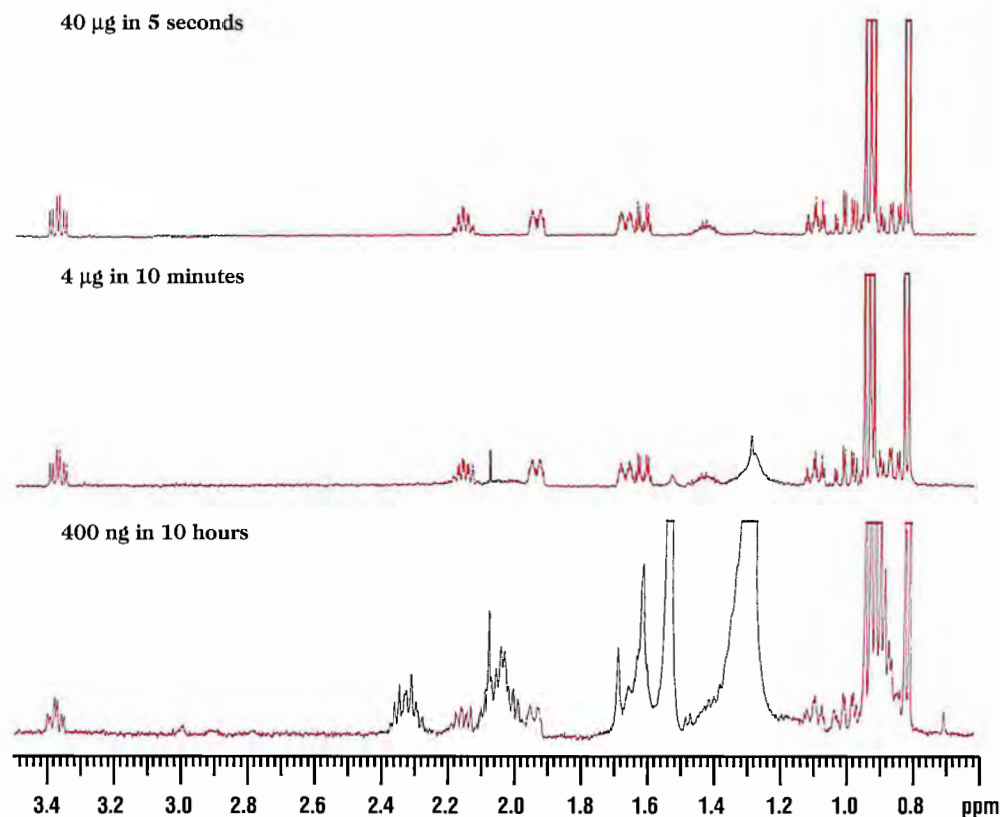
Polybutadiene-d₆

Figure 1b

Figure 1a



Detect Nanogram Quantities with Varian's New Probe Technology.



These spectra of menthol in CD₂Cl₂ were obtained on a UNITY 500 MHz spectrometer with the Nano•nmr probe™. The new peaks in the lower spectra (shown in black) are from solvent impurities.

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Varian leads the way with innovative probe technologies that open new realms in NMR spectroscopy. The Nano•nmr probe's unique design guarantees the highest sensitivity for minute quantities of sample which reduces acquisition times by more than an order of magnitude.

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Varian's Nano•nmr Probe Opens New Opportunities

Advantages

- Routinely detects μ gram quantities of sample and permits nanogram quantities to be studied.
- Achieves uniform excitation over broad spectral windows with short pulse widths.
- Obtains higher effective dynamic range and fewer solvent artifacts by using less solvent.
- Runs multi-dimensional structure determination experiments on small quantities of sample.
- Provides uncompromised high resolution results.

Applications

- Study of synthesized or isolated natural products.
- Analysis of metabolites that are available only in small quantities.
- Detection of minute quantities of impurities.
- Structure determination of synthetic intermediates.

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NEW CAMPUS DEDICATION

TAMU NMR Newsletter
Bernard L. Shapiro, Editor/Publisher
966 Elsinore Court
Palo Alto, CA 94303

OCTOBER 14, 1993

September 14, 1993
(received 9/23/93)

Dear Barry:

While "doing the demo circuit" last spring, we acquired some ^1H spectra of semisolid aqueous mixtures consisting of egg phosphatidylcholine (PC) and cholesterol (CH). The liquid-crystalline (multilamellar) nature of these samples gives their 300 MHz MAS spectra broad lines and diminished intensity in the acyl-chain methylene region; as observed previously there are no identifiable signals from the cholesterol component (Figure 1). Raising the spin rate to 4 kHz enhances the signal intensity in both methylene and methine regions of the spectrum; it even produces enough line narrowing to reveal artifacts from poor shimming (Figure 2) (!). Despite the semisolid nature of the PC-CH mixture, we were able to achieve a dramatic improvement in resolution through a somewhat unorthodox application of CRAMPS (Figure 3). Yet when all is said and done, the best results come from the brute force approach: provided that we can avoid sample heating and phase separation, simple 7 kHz MAS (^1H at 300 MHz, Figure 4) and 11 kHz (^1H at 400 MHz, Figure 5) yield the nicest spectra.

Can you guess which vendors belong to the various spectra?! We thank all parties concerned for permission to present these data.

Sincerely yours,

Ruth E. Stark
Professor of Chemistry

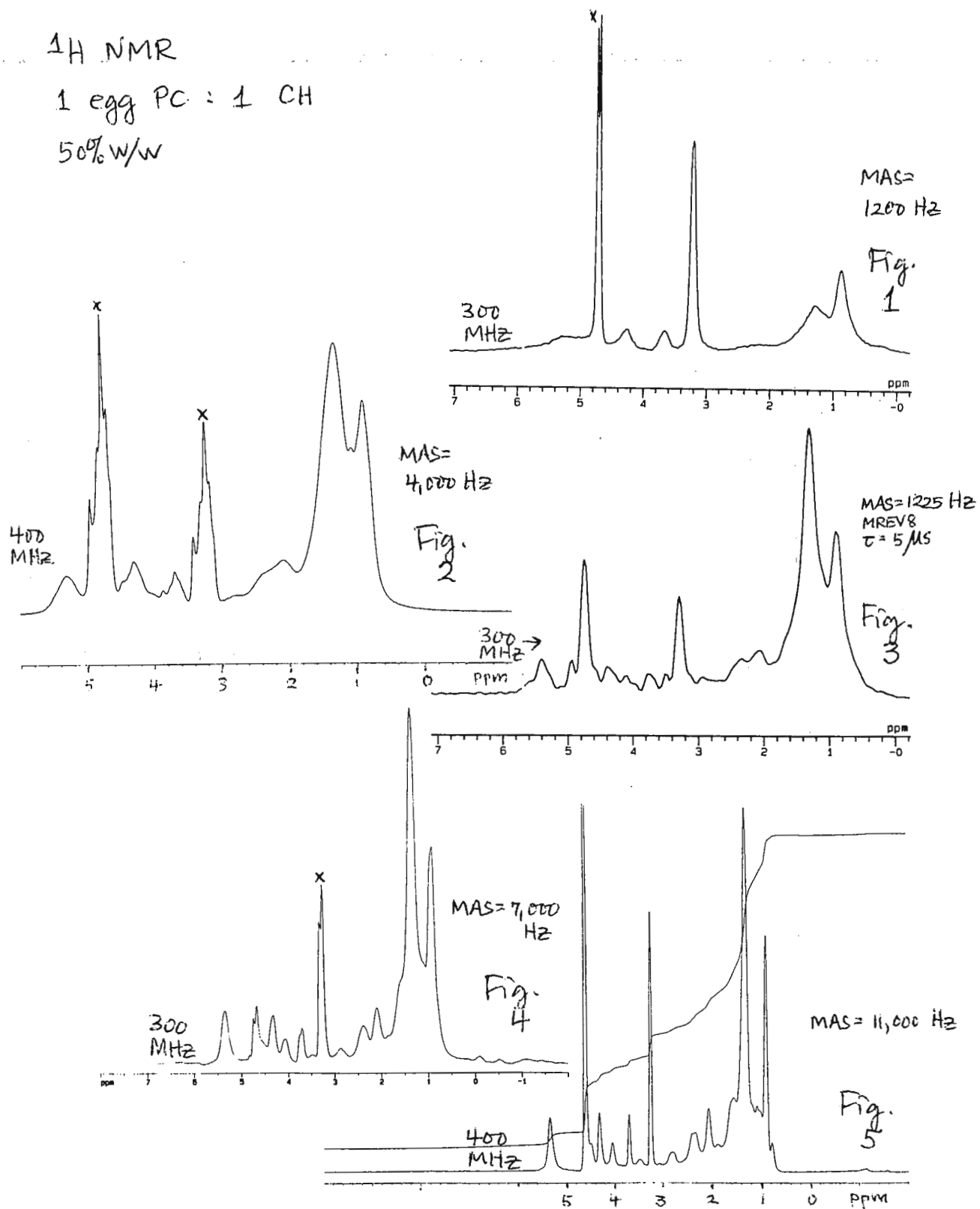
P.S. Please credit this contribution to the CUNY NMR account, which now resides with me at The College of Staten Island's brand new campus.

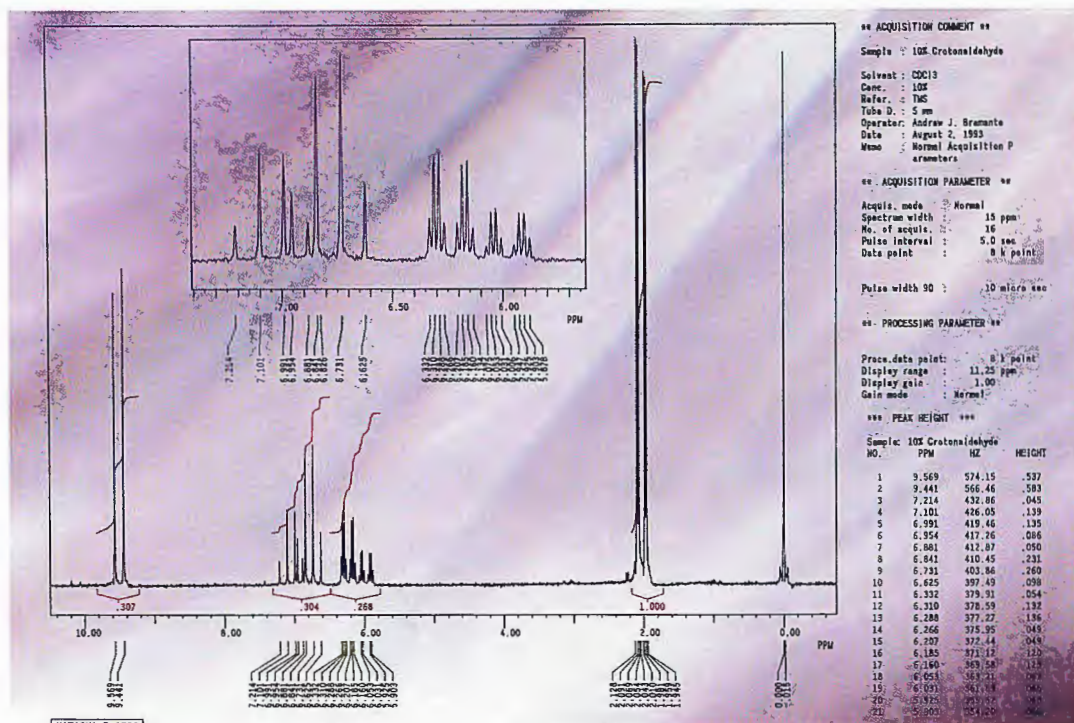
scratch tamu.let 091493

^1H NMR

1 egg PC : 1 CH

50% w/w





This R-1500 FT-NMR spectrum of crotonaldehyde represents a 16 pulse acquisition; each pulse was 10 μ sec with a pulse interval of 5 seconds.

HIGH RESOLUTION DIGITAL 60 MHz NMR. GET THE WHOLE STORY IN FIVE SECONDS.

Digital is the new wave in high-resolution 60 MHz NMR spectroscopy. That's because it's not only faster than old analog technology, but it extends the application beyond the acquisition of a simple spectrum. And only Hitachi has it.

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IF YES, PLEASE LIST MANUFACTURER AND MODEL: _____

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ARE YOU CONSIDERING AN NMR SPECTROMETER FOR PURCHASE?

Yes ☐ No ☐

IF YES, AT WHAT FIELD STRENGTH? _____

IF YES, WHEN DO YOU NEED IT? _____

HAVE YOU DISCUSSED YOUR APPLICATION(S)
WITH A HITACHI REPRESENTATIVE?

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August 24, 1993

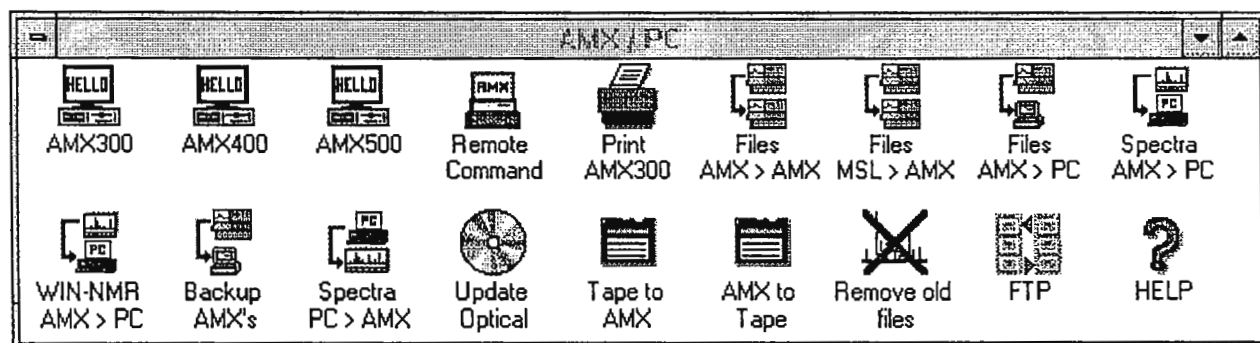
(received 9/11/93)

Dr. Bernard L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

Dear Barry:

Our laboratory has been undergoing extensive renovations which have included the acquisition of 3 Bruker AMX spectrometers (300, 400, and 500 MHz). The 300 and 500 have automated sample changers with which we have enjoyed many successes and as a result, a demanding workload. We have found the tape drive systems utterly inadequate as a means for archiving the data acquired due to the poor integrity and fortitude of the medium and the slow retrieval rate for that last file on the tape. To solve this problem with no substantial capital investment funding to do so, we have implemented a computer network using PC/TCP Network Software for MS-DOS or WINDOWS™ from FTP Software Inc.. This software, as many are aware, uses TCP/IP ethernet protocol, and we have found it extremely useful using both MS-DOS and Microsoft Windows™ operating environments in conjunction with the UNIX operating software of the NMRs. The physical network is comprised of AT&T 3COMM ethernet boards on the PCs and Bruker's ethernet card in their X-32 computer. Both boards have a BNC connector which allows for simple connection of the systems using Teflon-coated coaxial cable. A Bruker MSL-200 solids instrument is also connected to the network and uses Bruknet (in the presence of TCP/IP) to routinely transfer data to the AMX-400 for processing or archival.

Some time has been spent developing batch programs designed to allow the novice user to complete file operations without any knowledge of the FTP software. This was most easily accomplished using the WINDOWS™ version of FTP and establishing a network window which is shown below. Each icon in the window has an associated batch program which calls specific FTP routines, custom C language programs, or in combination to complete specific functions associated with it, such as file transferring, obtaining directories...etc. An example of a typical batch program for the transfer of data files from an AMX to a PC is also shown. With this system in place, we will be using a 486/66 PC with a 1 Gbyte local bus drive and a 600 Mbyte rewritable optical drive to archive the NMR spectra in a reliable manner. The use of a central

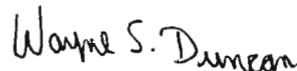


optical drive, in conjunction with WINDOWS for WorkGroups™, will allow NMR laboratory personnel to access the optical from their individual PCs as if it were resident on their own system and share peripherals resident on the various PCs. Several processing packages, including Bruker's WIN-NMR, Gramm's 386, and NUTS by Acorn NMR are being used on the PCs for spectral manipulation. At this point, it is possible to place the data in any number of WINDOWS™ graphical or desktop publishing applications for direct incorporation into articles or reports. While this system may not be as elegant as a full UNIX network with workstations, given the popularity of PCs and the relatively low cost of the network hardware and software, we have found this to be an inexpensive and very adaptable alternative.

Best Regards,



Thomas G. Neiss



Wayne S. Duncan

Batch Program for the transfer of data files from an AMX system to PC.

```
@ rem =====
@ echo off

rem ! File name : AMX2PC.BAT
rem ! Function  : Copy files from AMX to PC
rem ! Arguments : pc_destination amx_from amx_path file_spec
rem ! Calls     : msd.exe rcp.exe
rem ! Example   : amx2pc d:\amx amx400 /u/lab *
rem ! Copy all files (recursively) from the amx400, directory /u/lab
rem ! to the PC directory d:\amx\amx400\u\lab
rem ! msd.exe is a custom "Make Sub Directory" program for the PC

set area=%1\%2
c:\nmrlab\msd %area%%3
attrib r %area%\*.* /s
c:\pctcp\rcp r b root@%2:%3/%4 %area%%3
```


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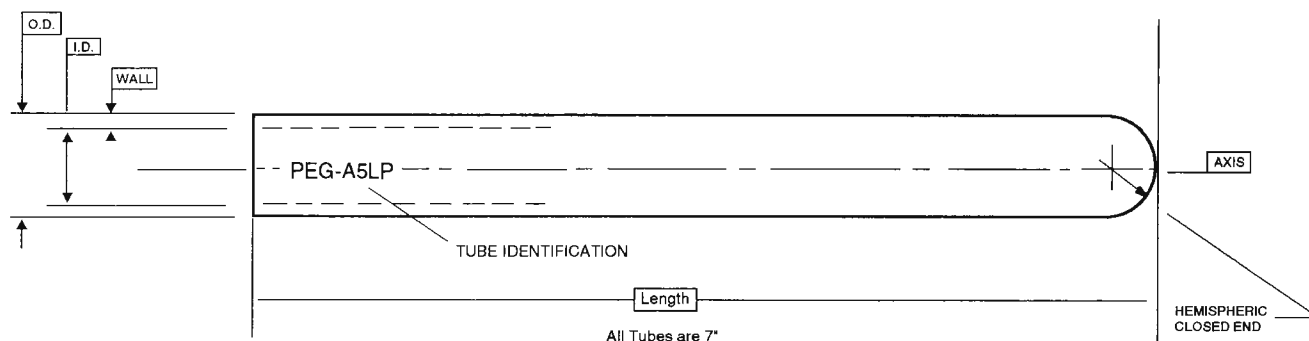
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16XXA5LP-07	>500	.1955	+.0000"/-.0005"	.1655	+.0005"/-.0000"	≤ .0005"	≤ .00025"
160XA5LP-07	360	.1955	+.0000"/-.0005"	.1655	+.0005"/-.0000"	≤ .0010"	≤ .0005"
1600A5LP-07	200	.1955	+.0000"/-.0005"	.1655	+.0005"/-.0000"	≤ .0015"	≤ .0010"
1600B5LP-07	150	.1955	+.0000"/-.0005"	.1655	+.0005"/-.0000"	≤ .0020"	≤ .0015"
1600C5LP-07	100	.1955	+.0000"/-.0005"	.1655	+.0005"/-.0000"	≤ .0020"	≤ .0020"
16XA10LP-07	360	.3937	+.0000"/-.0005"	.3569	±.0005"	≤ .0015"	≤ .0005"
160A10LP-07	150	.3937	+.0000"/-.0005"	.3569	±.0005"	≤ .0020"	≤ .0010"
160B10LP-07	80	.3937	+.0000"/-.0005"	.3569	±.0005"	≤ .0030"	≤ .0015"
160C10LP-07	60	.3937	+.0000"/-.0005"	.3569	±.0005"	≤ .0050"	≤ .0020"
DISPOSABLE NMR TUBES							
1600A5LS-07	80	.1955	+.0000"/-.0005"	.165	±.005	≤ .003	≤ .002
1600A5RS-07	60	.196	±.003	.165	±.005	≤ .005	≤ .002

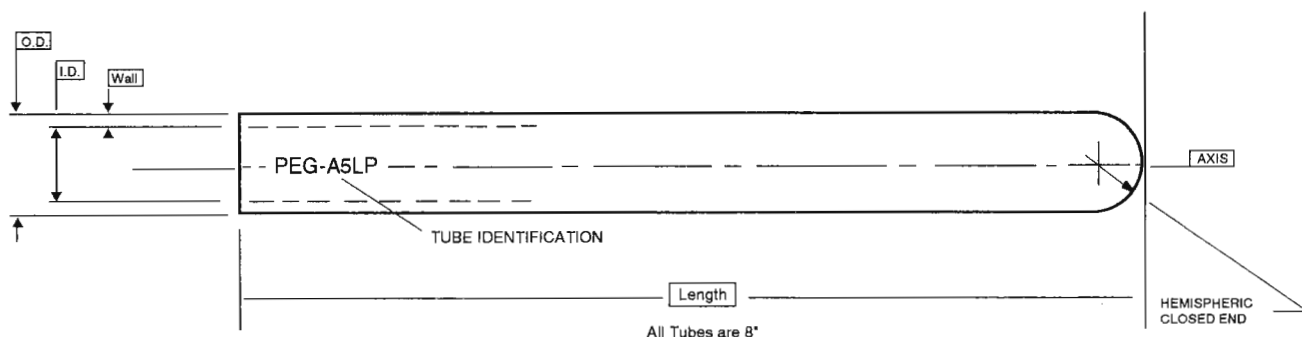
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All Tubes supplied in Package Quantity of 5 or 25 pieces.

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160XA5LP-07	5mm/7"	★43.25	★216.25
1600A5LP-07	5mm/7"	★37.00	★185.00
1600B5LP-07	5mm/7"	★27.50	★137.50
1600C5LP-07	5mm/7"	★22.50	★112.50
16XA10LP-07	10mm/7"	★93.75	★468.75
160A10LP-07	10mm/7"	★78.75	★393.75
160B10LP-07	10mm/7"	★68.00	★340.00
160C10LP-07	10mm/7"	★51.25	★256.25
1600A5LS-07	5mm/7"	★17.50	★ 87.50
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TUBE SPECIFICATIONS

5 and 10mm x 8" length



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16XXA5LP-08	>500	.1955	+ .0000"/- .0005"	.1655	+ .0005"/- .0000"	≤ .0005"	≤ .00025"
160XA5LP-08	360	.1955	+ .0000"/- .0005"	.1655	+ .0005"/- .0000"	≤ .0010"	≤ .0005"
1600A5LP-08	200	.1955	+ .0000"/- .0005"	.1655	+ .0005"/- .0000"	≤ .0015"	≤ .0010"
1600B5LP-08	150	.1955	+ .0000"/- .0005"	.1655	+ .0005"/- .0000"	≤ .0020"	≤ .0015"
1600C5LP-08	100	.1955	+ .0000"/- .0005"	.1655	+ .0005"/- .0000"	≤ .0020"	≤ .0020"
16XA10LP-08	360	.3937	+ .0000"/- .0005"	.3569	± .0005"	≤ .0015"	≤ .0005"
160A10LP-08	150	.3937	+ .0000"/- .0005"	.3569	± .0005"	≤ .0020"	≤ .0010"
160B10LP-08	80	.3937	+ .0000"/- .0005"	.3569	± .0005"	≤ .0030"	≤ .0015"
160C10LP-08	60	.3937	+ .0000"/- .0005"	.3569	± .0005"	≤ .0050"	≤ .0020"
DISPOSABLE NMR TUBES							
1600A5LS-08	80	.1955	+ .0000"/- .0005"	.165	± .005	≤ .003	≤ .002
1600A5RS-08	60	.196	± .003	.165	± .005	≤ .005	≤ .002

All Tubes are 8" long. Other sizes are available, phone for information.

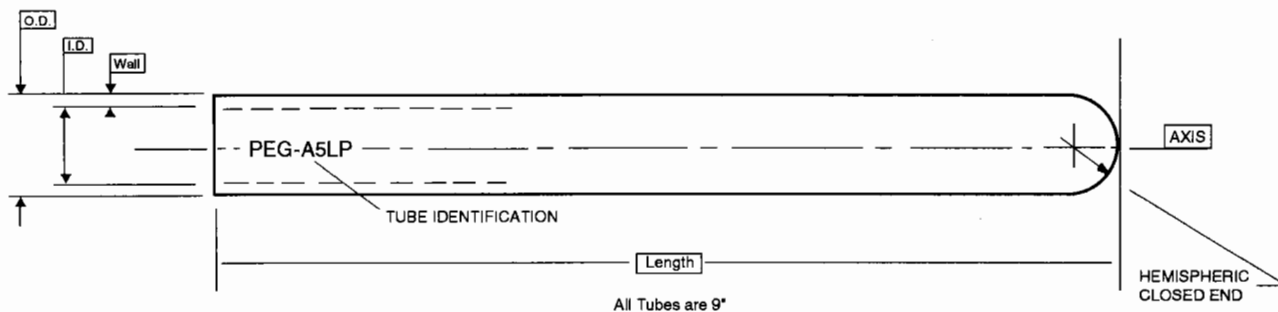
All Tubes supplied in Package Quantity of 5 or 25 pieces.

ACE Catalog No.	Tube Size O.D./Length	Per Pkg./5	Per Pkg./25
16XXA5LP-08	5mm/8"	★64.75	★323.75
160XA5LP-08	5mm/8"	★47.75	★238.75
1600A5LP-08	5mm/8"	★40.75	★203.75
1600B5LP-08	5mm/8"	★30.25	★151.25
1600C5LP-08	5mm/8"	★24.75	★123.75
16XA10LP-08	10mm/8"	★97.50	★487.50
160A10LP-08	10mm/8"	★83.75	★418.75
160B10LP-08	10mm/8"	★72.25	★361.25
160C10LP-08	10mm/8"	★56.25	★281.25
1600A5LS-08	5mm/8"	★19.25	★ 96.25
1600A5RS-08	5mm/8"	★ 8.50	★ 42.50

★ Net

TUBE SPECIFICATIONS

5 and 10mm x 9" length



ACE Cat. No.	Megahertz (MHz) Inst. Frequency	O.D. inches	O.D. Tolerance	I.D. inches	I.D. Tolerance	Concentricity I.D. to O.D.	Camber (Over 9" Lgth.)
16XXA5LP-09	>500	.1955	+ .0000" / - .0005"	.1655	+ .0005" / - .0000"	≤ .0005"	≤ .00025"
160XA5LP-09	360	.1955	+ .0000" / - .0005"	.1655	+ .0005" / - .0000"	≤ .0010"	≤ .0005"
1600A5LP-09	200	.1955	+ .0000" / - .0005"	.1655	+ .0005" / - .0000"	≤ .0015"	≤ .0010"
1600B5LP-09	150	.1955	+ .0000" / - .0005"	.1655	+ .0005" / - .0000"	≤ .0020"	≤ .0015"
1600C5LP-09	100	.1955	+ .0000" / - .0005"	.1655	+ .0005" / - .0000"	≤ .0020"	≤ .0020"
16XA10LP-09	360	.3937	+ .0000" / - .0005"	.3569	± .0005"	≤ .0015"	≤ .0005"
160A10LP-09	150	.3937	+ .0000" / - .0005"	.3569	± .0005"	≤ .0020"	≤ .0010"
160B10LP-09	80	.3937	+ .0000" / - .0005"	.3569	± .0005"	≤ .0030"	≤ .0015"
160C10LP-09	60	.3937	+ .0000" / - .0005"	.3569	± .0005"	≤ .0050"	≤ .0020"
DISPOSABLE NMR TUBES							
1600A5LS-09	80	.1955	+ .0000" / - .0005"	.165	± .005	≤ .003	≤ .002
1600A5RS-09	60	.196	± .003	.165	± .005	≤ .005	≤ .002

All Tubes are 9" long. Other sizes are available, phone for information. All Tubes supplied in Package Quantity of 5 or 25 pieces.

ACE Catalog No.	Tube Size O.D./Length	Per Pkg./5	Per Pkg./25
16XXA5LP-09	5mm/9"	★ 71.25	★ 356.25
160XA5LP-09	5mm/9"	★ 52.50	★ 262.50
1600A5LP-09	5mm/9"	★ 45.00	★ 225.00
1600B5LP-09	5mm/9"	★ 33.25	★ 166.25
1600C5LP-09	5mm/9"	★ 27.25	★ 136.25
16XA10LP-09	10mm/9"	★ 101.75	★ 506.25
160A10LP-09	10mm/9"	★ 88.75	★ 443.75
160B10LP-09	10mm/9"	★ 76.50	★ 382.50
160C10LP-09	10mm/9"	★ 62.00	★ 310.00
1600A5LS-09	5mm/9"	★ 22.25	★ 111.25
1600A5RS-09	5mm/9"	★ 9.00	★ 45.00

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August 19, 1993 (received 8/23/93)

Dr. Bernard Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

ANATOMY (NMR) OF A TROUT FLY

Dear Barry:

Seems that every time we get your notice about a contribution our minds are on other things. This time we were in the process of tying flies while waiting for the runoff to end and for Wyoming's one day of summer to start, which we haven't had yet. We have a saying in Wyoming that the way to a man's heart is through his fly. Um, ah, er- trout fly that is. So we thought the readers would like to see what the anatomy of a trout fly looks like using NMR.

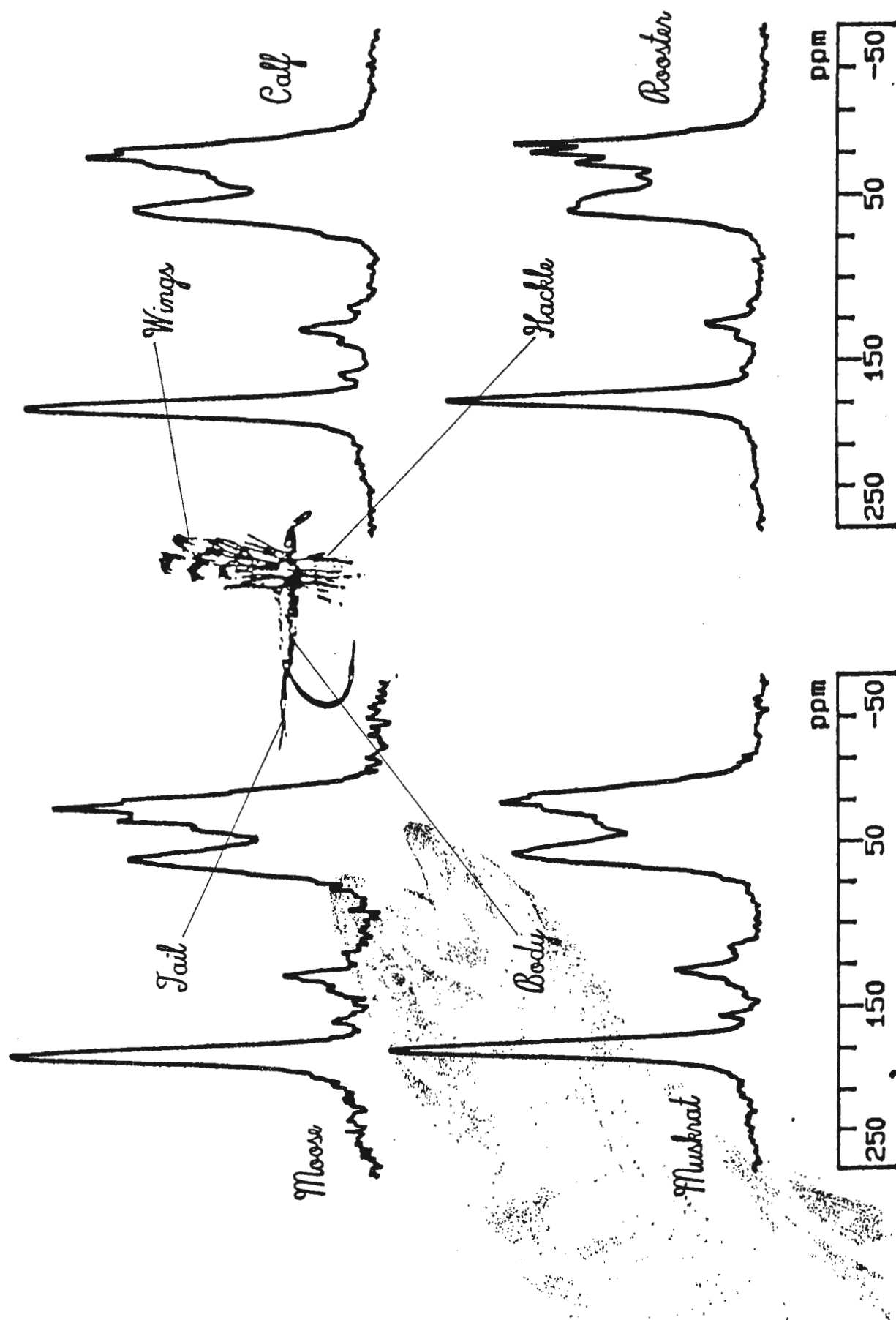
The CP/MAS ^{13}C NMR spectra in the figure represent the various materials that comprise a popular trout fly known as an Adams, only we have taken the liberty to modify it slightly by including calf tail fur for the wing instead of feathers. The fly dressing consists of: moose body hair for the tail, muskrat fur for the body, calf tail for the wings, and Plymouth rock rooster feathers for the hackle. Despite the different kinds of animal materials making up the fly, the NMR spectra of all the materials are primarily those of keratin, a fibrous protein. There are only slight differences among the spectra of the furs. The most noticeable difference is between the furs and the feather where the spectrum of the feather has greater resolution of aliphatic carbons. Fortunately, fish don't discriminate as well as NMR does, and all of it looks good to the trout.

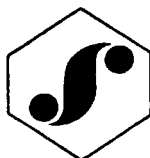
Well, we're off to test our creation in the field. NMR can only do so much. Sometimes one has to put things to the test. Ah, but that's what life is all about, at least here in Wyoming.

Best regards,

Fran Miknis

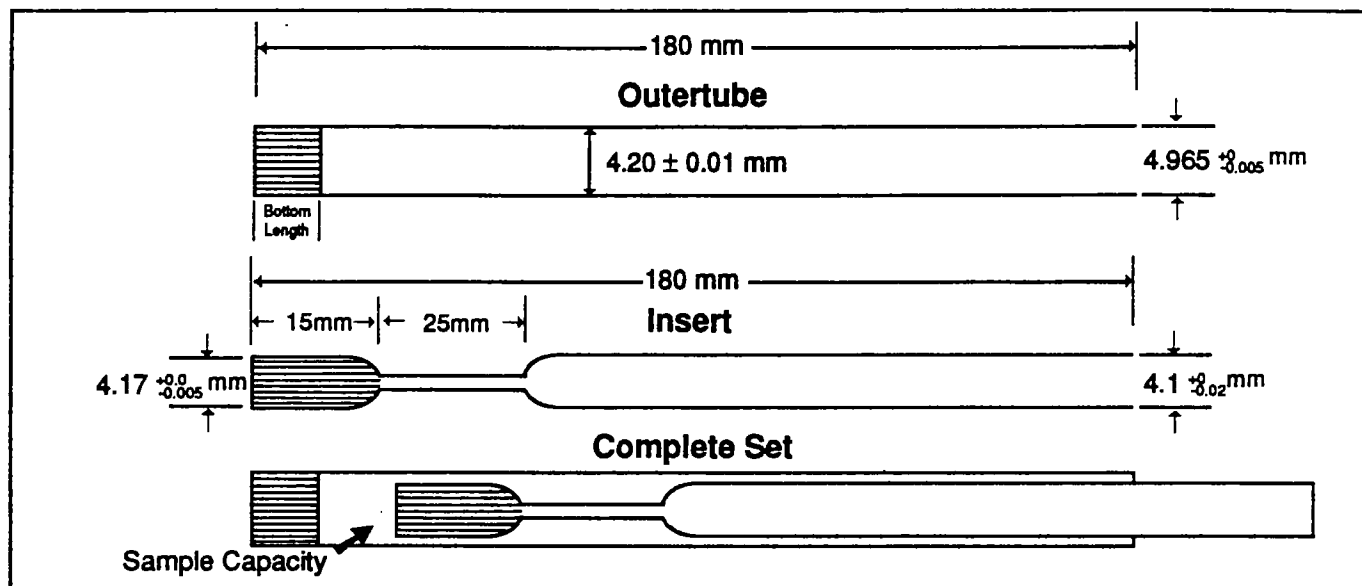
Dan Netzel





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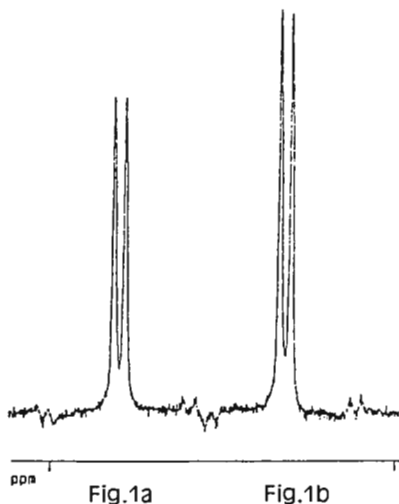
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	(mm)				ID (mm)	OD (mm)	
BMS-005B	180	2.6	4.1	180	4.2	4.965	8
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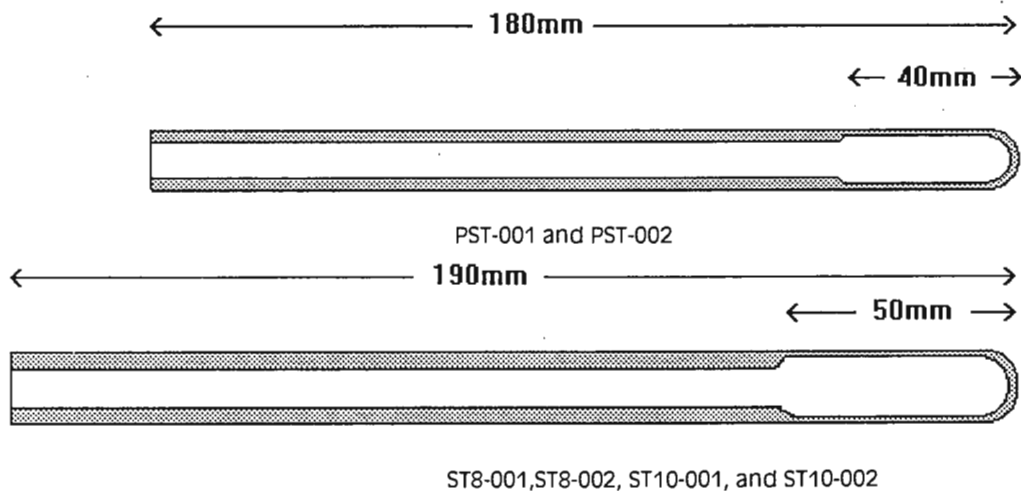
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8.0	ST8-001	0.25	40/ 8	8.00 + 0.00 - 0.01	7.52 ± 0.01
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	ST10-002	0.25	50/15		

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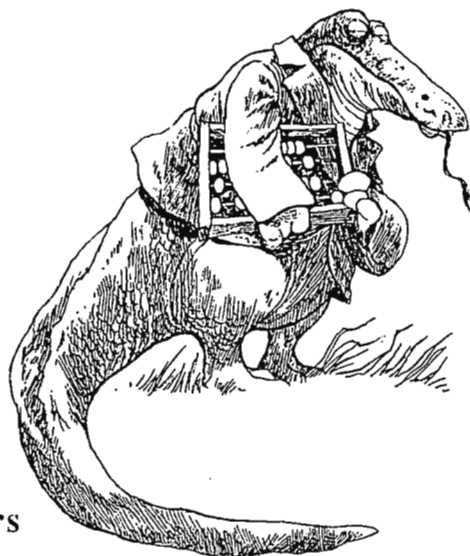
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UNIVERSITY OF CAMBRIDGE
DEPARTMENT OF CHEMISTRY
Lensfield Road, Cambridge, U.K.

Professor Barry Shapiro,
Editor, TAMU Newsletter,
Elsinor Court,
Palo Alto,
California 94303 USA

6 . ix . 93
(received XI/09/XCIII)



Dear Barry,

Early Jurassic Digital Computers

I never quite understood how one manages to do long division on an abacus but I can imagine it can cause real difficulties when the denominator is zero. There were similar problems with digital computers in the 1960's; they seemed to blow all their fuses in this situation. Later computers checked one's arithmetic beforehand and sent a rather shirty error message. Division by zero was a crime almost as unforgivable as using double spacing in the Newsletter. *

Now there is a nice experiment suggested by Axel Bothner-By and Joe Dadok¹ where they deconvolute J-splittings from individual spin multiplets by dividing the corresponding time-domain signal by $\cos(\pi J^* t)$ where J^* is a trial coupling constant. Problems arise when the cosine wave is zero or near zero. Because of these numerical instabilities, a considerable amount of research has gone into alternative methods of deconvolution that avoid this problem. For example, we once advocated a method that carefully sampled the cosine wave in such a manner as to avoid the zero-crossings.²

We have recently attacked this problem again from another angle. In this particular case the cosine wave is a noisy signal which makes the problem even trickier. We test each ordinate of the time-domain denominator to see if its modulus is less than a predefined threshold θ . If it is, it is replaced by θ , retaining the original sign. A good value of θ seems to be something comparable with the peak-to-peak noise level, but in fact the method is surprisingly tolerant of the choice of θ (over several orders of magnitude). It even works when θ is so high that all the ordinates are replaced by $+\theta$ or $-\theta$ although in this case there are complications due to harmonics of the basic frequency. After division, any residual spikes in the quotient can be smoothed by a simple 1:2:1 convolution algorithm, repeated if necessary. We think that this might be one of the simplest solutions to the J-deconvolution problem.

Kindest regards,

Ray

Ray Freeman

¹ A. A. Bothner-By and J. Dadok, *J. Magn. Reson.* 72, 540 (1987).

² J. M. Le Parco, L. McIntyre and R. Freeman, *J. Magn. Reson.* 97, 553 (1992).

*Or misspelling Aksel, or leaving the last letter off Elsinore.

Thanks, Roy.

BLS.



DEPARTMENT OF CHEMISTRY
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9/01/93

(received 9/7/93)

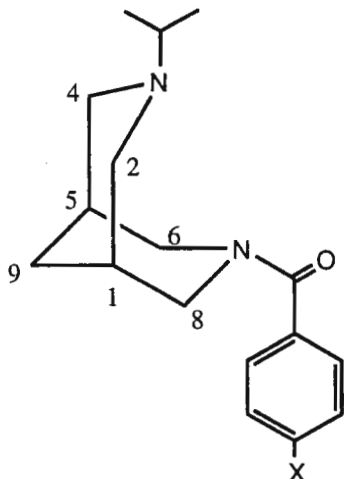
Dr. B L. Shapiro
966 Elsinore Court
Palo Alto, CA 94303

Title: Amides of Bispidines

Dear Barry:

In our recent work we have had occasion to prepare some bispidines with amide linkages. We thought it interesting to note the dramatic effect of a fluorine atom on long distance chemical shifts in such systems as shown below with the two examples. We have not been able to separate and identify all of the signals from

Group	X (ppm from TMS)	
	NO ₂	F
(H ₃ C) ₂	0.56/0.69	0.96/1.07
H(9) _{ax}	1.34	1.71 [+ H(5)]
H(1)	1.64	1.95
3 H	3.04-2.32	2.41-2.72 [4 H]
2 H	2.67	3.03
1 H	2.94	3.31
1 H	3.20	3.72
1 H	3.39	4.74



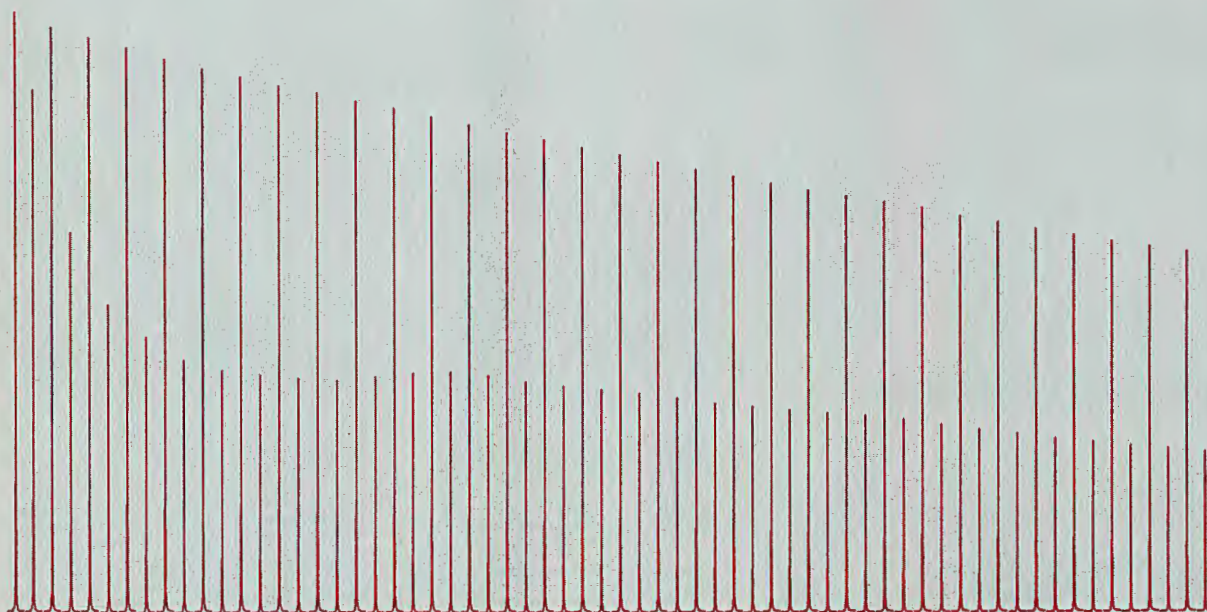
the spectra taken on our XL-400 NMR spectrometer. There is, of course, considerable nonequivalence of protons because of the amide linkage as expected. This is clearly demonstrated by the nonequivalence of the protons on the methyl groups in the isopropyl function. Obviously, there is also nonequivalence in most of the ring protons which makes assignment of those signals very difficult even with decoupling. We are in the process of performing other experiments to attempt to unravel the signal patterns since this field has very few model systems available for any comparison purposes.

One half of our NMR capability has been disabled of late and thus our productivity has been reduced significantly. We trust the above discussion will serve as our contribution. Best regards.

Sincerely yours,

K. Darrell Berlin
Regents Professor

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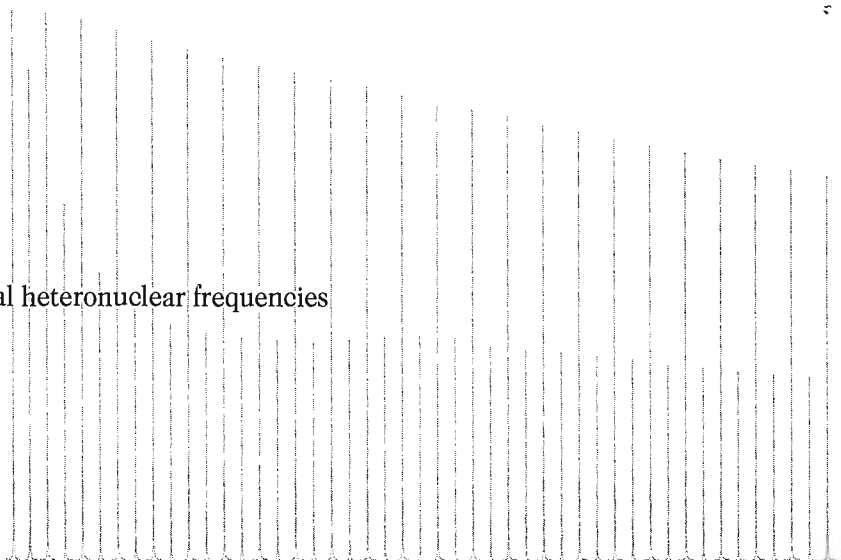
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DEPARTMENT OF THE NAVY
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IN REPLY REFER TO:

5 August 1993 (received 9/13/93)

"'ALL RIGHT,' SAID THE CAT; AND THIS TIME IT VANISHED QUITE SLOWLY, BEGINNING WITH THE END OF THE TAIL, AND ENDING WITH THE GRIN, WHICH REMAINED SOME TIME AFTER THE REST OF IT HAD GONE." (Lewis Carroll, *Alice in Wonderland*)

Dear Barry:

A number of groups are trying to better understand the growth of multiple-quantum NMR coherences in the extended spin systems characteristic of many solids. A one-dimensional chain of uniformly-spaced spin-1/2 nuclei represents the simplest example of such "infinite" spin systems; the ^1H and ^{19}F nuclei of calcium hydroxyapatite and fluorapatite represent close approximations to this ideal. From the ^1H phase-incremented MQ-NMR of polycrystalline hydroxyapatite we have observed that the effective size N of the spin system initially increases linearly with the multiple-quantum preparation time, in accord with the predicted effects of dimensionality in the model of Levy and Gleason. In order to eliminate possible undesirable effects from the powder averaging in this experiment, we decided to try to select specific crystallite orientations in a polycrystalline sample of fluorapatite, $\text{Ca}_5\text{F}(\text{PO}_4)_3$, relying upon the alignment of the axially-symmetric ^{19}F CSA tensor ($\Delta\sigma = 84$ ppm) along the chain axis of the dipolar couplings.

Chemical-shift selectivity in phase-incremented MQ-NMR cannot be achieved using familiar hard-pulse strategies, because of the distribution of overlapping homogeneous linewidths. Instead, we use a series of stepped-frequency weak (compared to the local fields) rf pulses, whose effects are in general described by the Provotorov equations. Experimental optimization allows fairly complete saturation of all but the homogeneously-broadened peak at the desired chemical shift, whose intensity is only slightly reduced. The normal MQ-NMR sequence is then applied, as shown in the left Figure. A strained attempt at acronymifying yielded only "CHEmical SHIf Removal Experiment," which promptly suggested the famous Cat referred to in the quote above, and its surprisingly appropriate behavior.

The effectiveness of this chemical-shift-selective MQ-NMR sequence is demonstrated by results for two different orientations of the fluorapatite chains, $\theta = 90^\circ$ and $\theta = 67^\circ$, which should have intrachain dipolar couplings in the ratio of 2:1. The slopes of the growth curves (N vs. MQ preparation time) shown in the right Figure are in the correct ratio. Furthermore, they scale (taking into account magnetogyric ratios and powder average dipolar couplings) with the results we previously obtained for hydroxyapatite (*Chem. Phys. Lett.*, **205**, 1, 1993), and thus help confirm the reliability of our comparisons with theory.

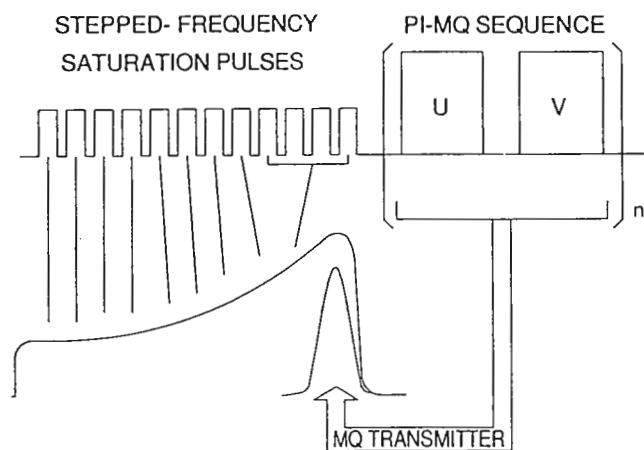
There are also additional interesting consequences of chemical-shift selectivity in MQ-NMR that we have demonstrated and are submitting for publication.

Sincerely yours,

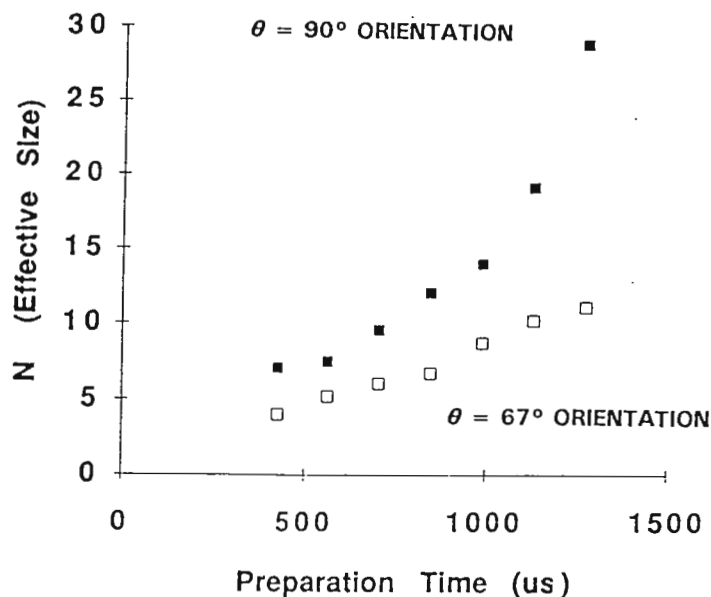
L.B.M.

Liam B. Moran
Department of Chemistry,
Michigan State University

James P. Yesinowski
Materials Chemistry Branch,
NRL



CHEMical SHift Removal Experiment (CHESHIRE)
for Phase-Incremented Multiple-Quantum NMR



Effective Size N vs. Preparation Time τ for
Two Different Crystallite Orientations in
Polycrystalline Fluorapatite

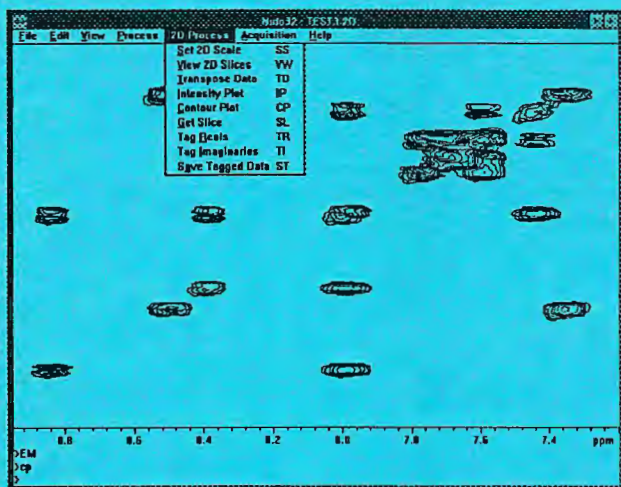
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Please contact:

Peter J. Domaille
E328/B50, DMPC
PO Box 80328
Wilmington, DE 19880-0328
Phone (302) 695-4916; FAX (302) 695-1128

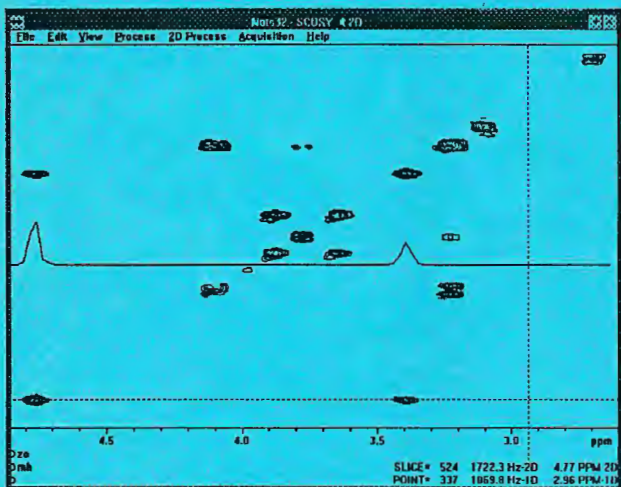
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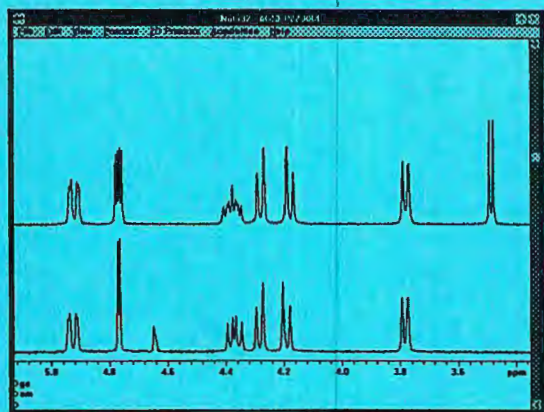
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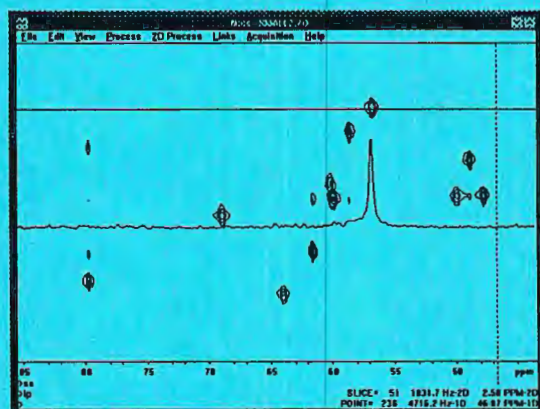
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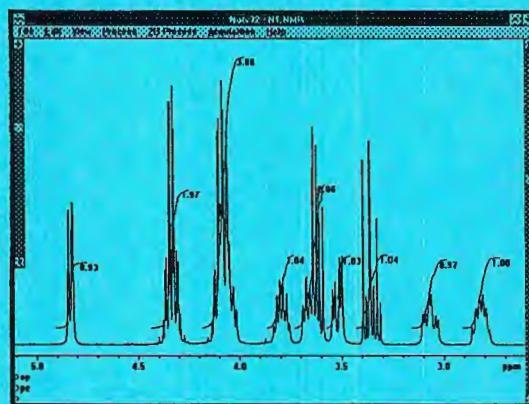
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September 16, 1993
(received 9/20/93)

Dr. Bernard L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

Selective Saturation of Broad Resonances in ^{31}P NMR Spectra *in vivo*

Dear Dr. Shapiro:

Broad resonances that lie underneath the familiar small molecule profile of *in vivo* ^{31}P NMR spectra can make accurate spectral integration of these mobile phosphates difficult. The two major broad components are the phosphate contained in the hydroxyapatite in cranial bone and the phosphodiester moiety in partially-mobile membrane phospholipids. They can be removed with post-acquisition processing but this results in distortion of lineshapes and intensities and interferes with accurate quantitation. We have implemented a selective off-resonance saturation procedure used previously in animal brains studies. Three advantages of this technique are: removal of the bone resonance, removal of the phospholipid resonance, and observation of the phospholipid resonance using spectral subtraction.

The bone resonance is extremely broad ($\sim 3.5\text{KHz}$ -120ppm) and makes up roughly 80% of the entire phosphorous signal from the head. The resonance is substantially reduced by applying a 200 msec gaussian pulse (4.5 watts, 0.5ppm bandwidth) 1090 Hz downfield from the phosphocreatine (PCr) peak before the excitation pulse. The bone resonance is a powder pattern whose shape is dominated primarily by chemical shift anisotropy. Uniform saturation is possible because the line is *homogeneously* broadened due to extensive $^1\text{H}/^{31}\text{P}$ heteronuclear dipole-dipole coupling. Saturation of the bone resonance effectively removes baseline distortion without affecting the sharp metabolites and is effective in baseline flattening in localized spectra acquired with chemical shift imaging (CSI) techniques.

Removal of the phospholipid peak is accomplished with a gaussian saturation pulse (same parameters as above) 290 Hz downfield from PCr. This technique along with ^1H decoupling and NOE enhancement greatly enhances the clarity of the peaks downfield from PCr. The off-resonance location and power of the saturation pulse were chosen to remove the maximum amount of phospholipid peak area and not compromise any of the signal from the phosphomonoester (PME) peaks which are the closest to the off-resonance pulse. Figure 1 shows a non-localized ^{31}P NMR spectra of the human head *in vivo*. The insert shows a shoulder (*) on the inorganic phosphate peak which corresponds to a region of pH 7.4.

Subtracting 290 Hz saturated data from 1090 Hz data yields a phospholipid peak very similar in appearance to the ^{31}P NMR spectra of multilamellar vesicles of L- α -phosphatidylcholine. 3D-CSI techniques can be used to create a localized phospholipid profile of the entire brain simultaneously. A 290 Hz 4D-CSI data set is subtracted from a 1090 Hz data set before Fourier transformation in the three spatial dimensions. The resulting information provides localized information about the relative phospholipid contribution. Monitoring localized phospholipid concentration may be important in studying tumor growth and demyelinating diseases.

Sincerely,

Ronald McNamara

Ronald McNamara

Fernando Arias-Mendoza

Truman R. Brown

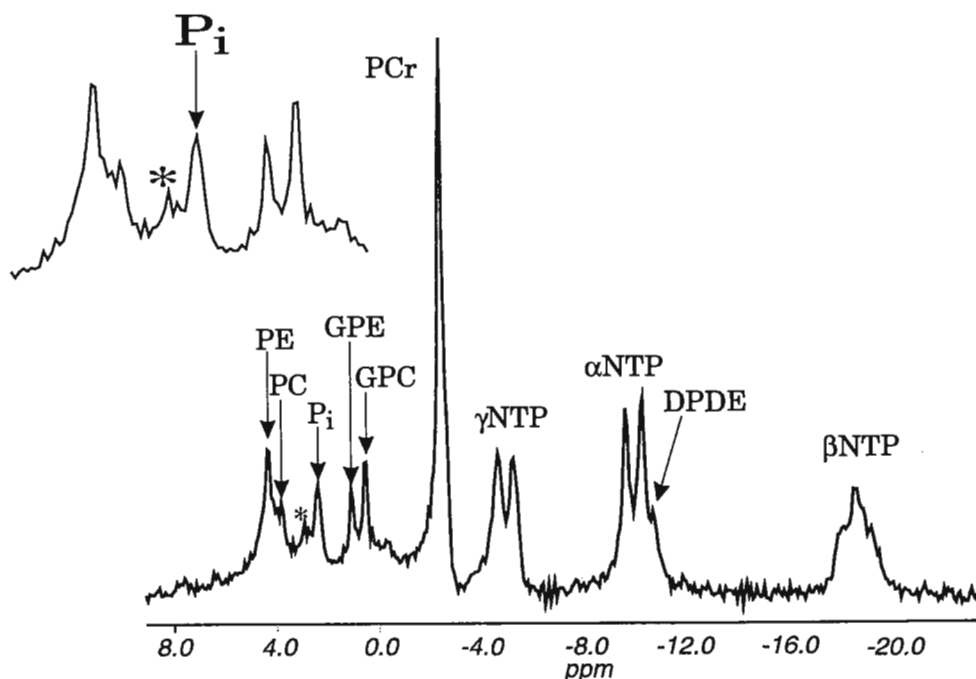
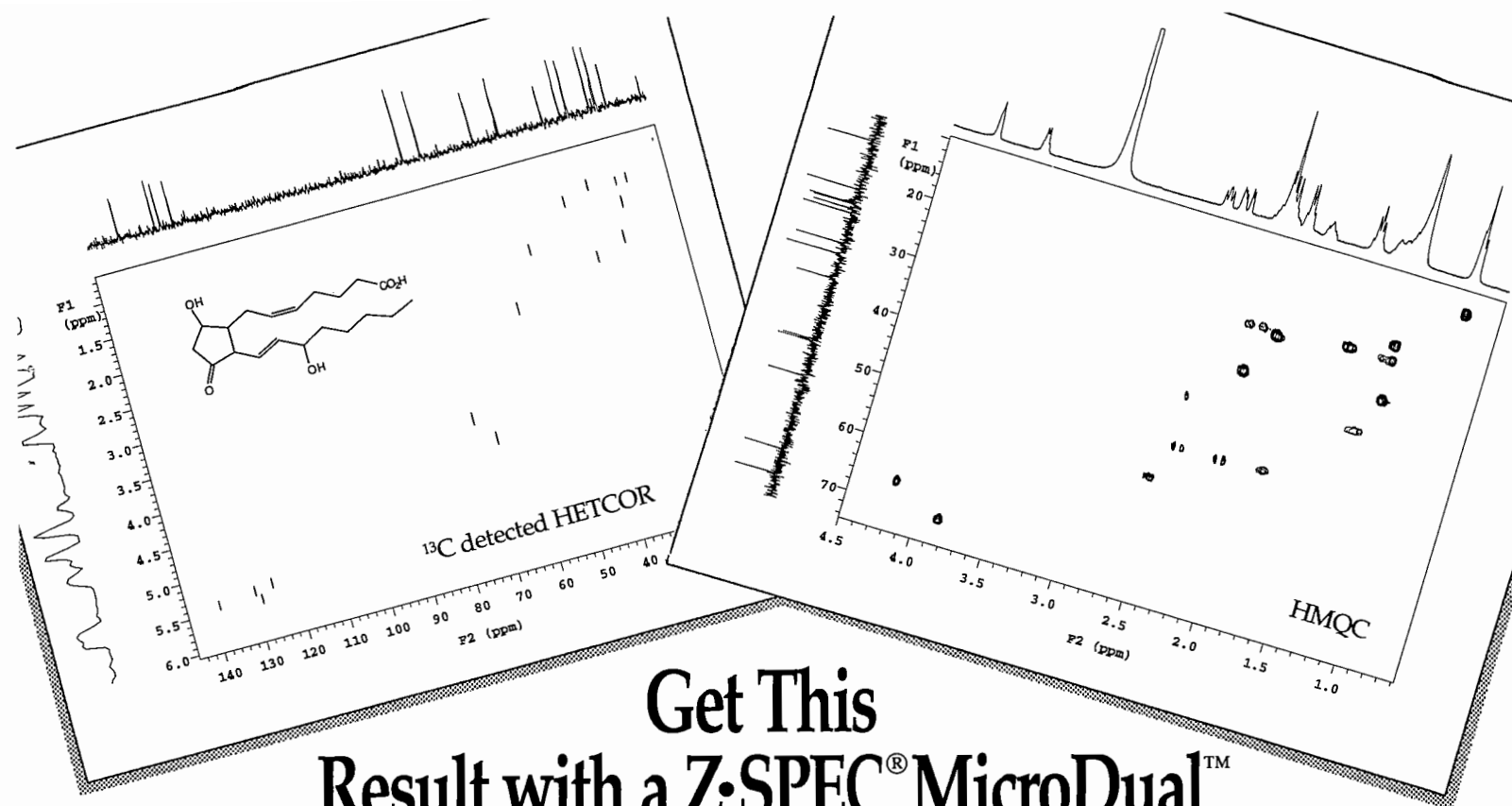


Figure 1



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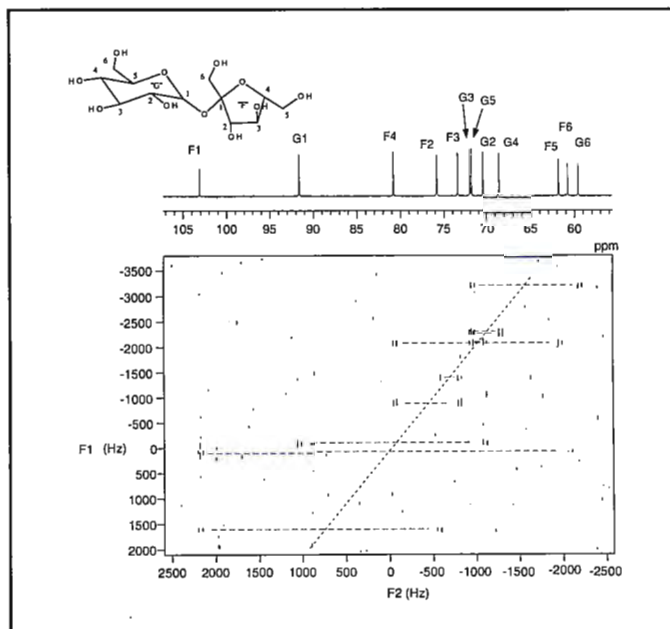


Figure 1: Phase-sensitive INADEQUATE spectrum acquired in 18 hours with 42mg Sucrose sample and Z•SPEC MD 400 probe.

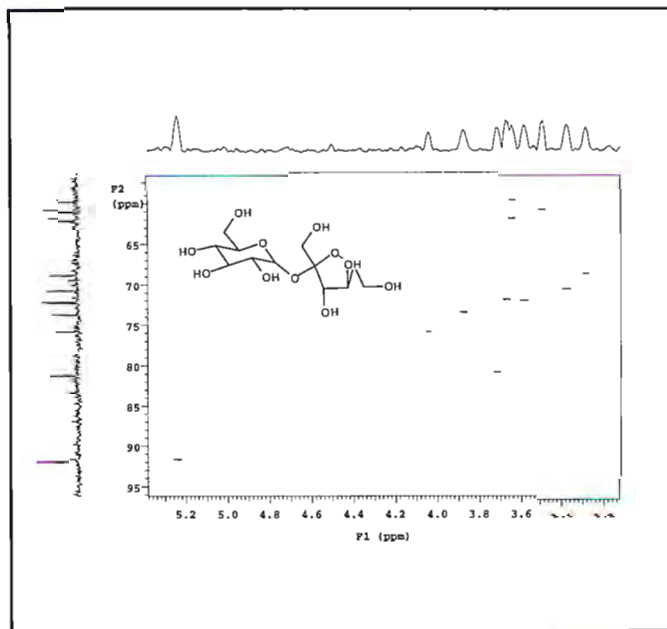


Figure 2: Phase-sensitive HETCOR spectrum of 600µg Sucrose acquired in 2 hours with a Z•SPEC MD 400 probe.

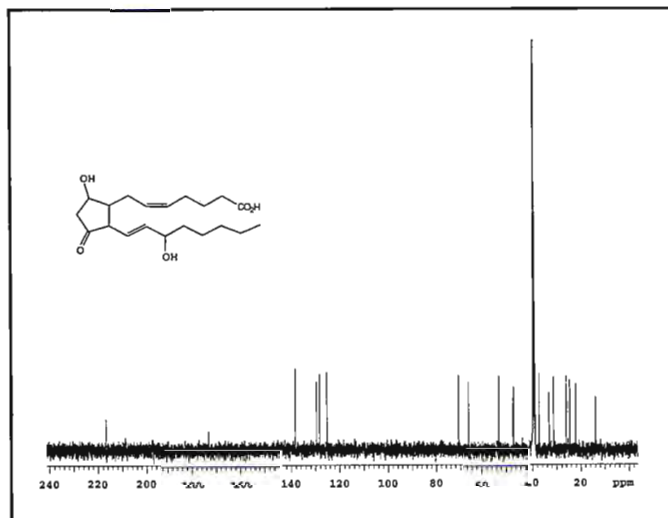


Figure 3: ^{13}C spectrum of 1.0mg Prostaglandin D2 obtained in 2 hours with a Z•SPEC MD 400 probe.

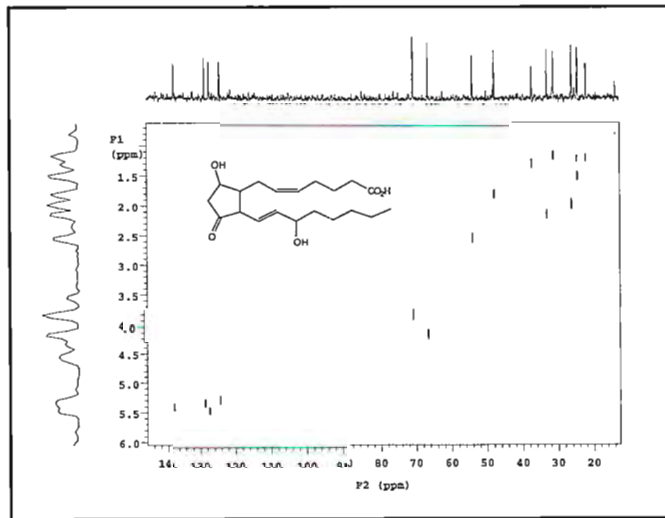


Figure 4: HETCOR of 1.0mg Prostaglandin D2 obtained in 14 hours with a Z•SPEC MD 400 probe.



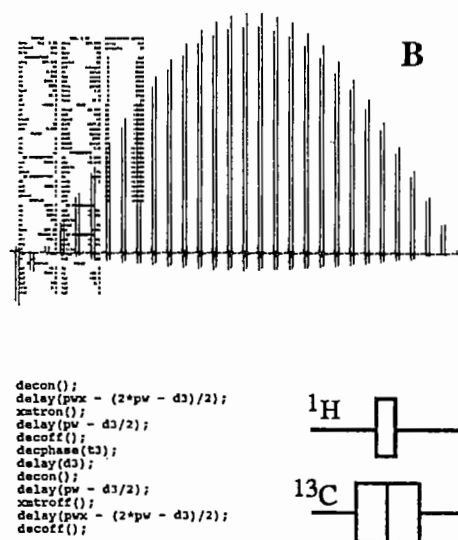
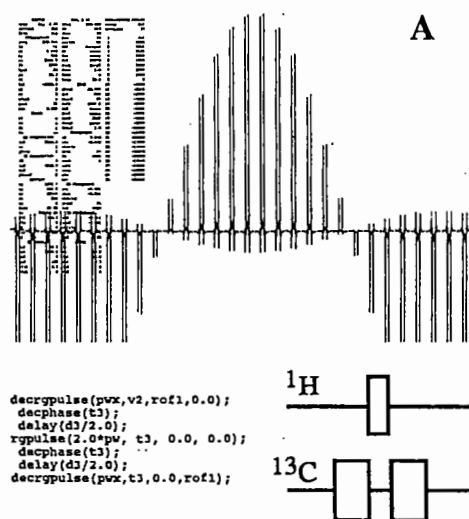
Dr. Bernard L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

September 8, 1993
(received 9/17/93)

Proper HMQC coding in multidimensional experiments.

Dear Barry,

We have been implementing a series of heteronuclear multidimensional experiments on our spectrometers, often starting from the code of related experiments. When we coded the ^{13}C -NOESYHMQC, we used the ^{15}N -NOESYHMQC code as a starting point, knowing that the ^{15}N experiment was working properly. However, after acquiring the first increment (^{13}C evolution time = 0) of the ^{13}C -NOESYHMQC on a protein sample, the FT clearly indicated a non-homogeneous ^{13}C excitation. We determined the ^{13}C excitation profile (fig. A, top) of the pulse sequence on a ^{13}C -glycine sample. The profile shows the first excitation nulls at ± 6000 Hz relative to the ^{13}C carrier frequency, approximately half the value obtained when doing the same calibration with the 2D-HMQC sequence. This reduced excitation profile is due to the way the HMQC 90-180-90 pulses are performed when the ^{13}C evolution delay (d3) is shorter than the proton 180° ($2 \cdot \text{pw}$). The code generating the HMQC section of the pulse sequence is shown at the bottom of figure A, along with the corresponding pulse representation. If the consecutive pulses are replaced by an overlapping scheme when $d3 < 2 \cdot \text{pw}$, as represented at the bottom of figure B, the correct excitation profile is obtained (fig. B, top). Note that for the ^{15}N -NOESYHMQC, the problem is usually not observed, due to relatively narrow spectral dispersion of nitrogen in proteins (on a 600MHz, ~ 1800 Hz for ^{15}N compared to ~ 9000 Hz for ^{13}C).



Stéphane M. Gagné
Stéphane M. Gagné

Brian D. Sykes
Brian D. Sykes

Announcing.....

GORDON CONFERENCE ON ORDER/DISORDER IN SOLIDS
"Frontiers of Science"

August 7-12, 1994
Colby-Sawyer College, New London, New Hampshire

Chair: Mary Anne White, Dalhousie University
Vice-Chair: Werner Press, Universität Kiel

The underlying theme of this Conference is order and disorder in condensed matter. The history of this Conference is distinguished: It started as "Plastic Crystals and Molecular Freedom" in January, 1976. The name was changed in 1978 to "Orientational Disorder in Crystals", and in 1988 to "Order/Disorder in Solids". Over the years, the emphasis has moved from "plastic crystals" to also include surfaces and interfaces, tunneling, incommensurate systems, inclusion compounds, glasses and, most recently, the C₆₀ family. The Conference has been particularly successful at bringing together chemists and physicists, experimentalists and theoreticians.

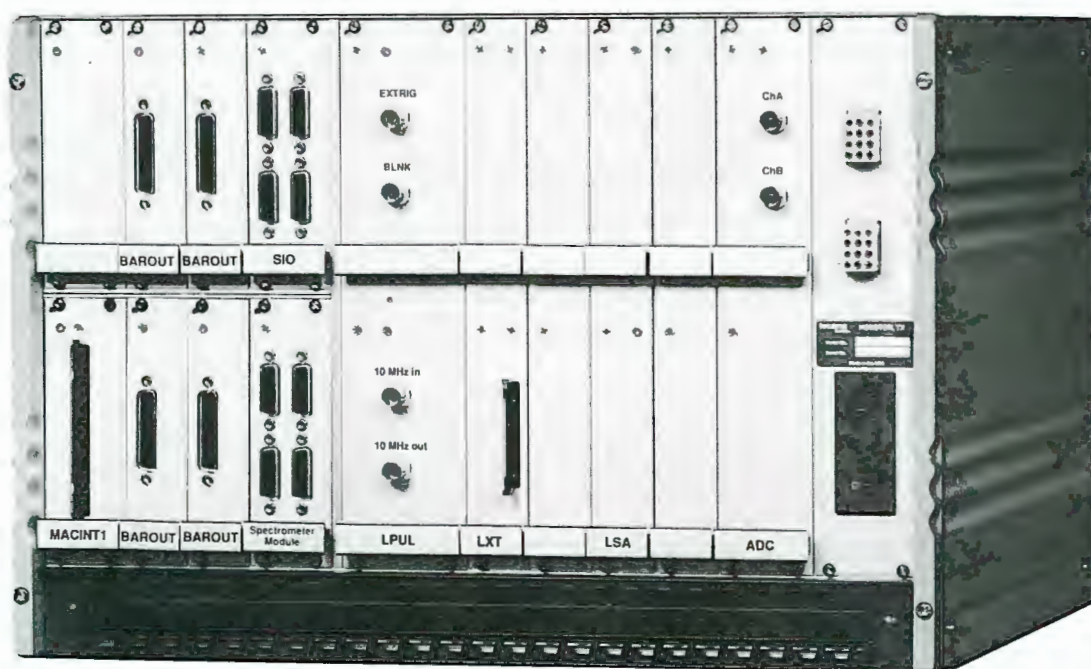
The scientific program for the 1994 Conference will consist of about 20 invited lectures in the field of disordered solids. In addition, there will be contributed posters and discussion groups. Topics to be included are: Fullerenes and molecular crystals; glasses; films and interfaces; tunneling; incommensurate systems; inclusion compounds. Techniques discussed will include nmr, Raman and other vibrational spectroscopies, light scattering, neutron and x-ray diffraction, thermodynamics, molecular dynamics, other aspects of theory. In keeping with the Gordon Research Conference philosophy, presentations will focus on current work, and attendance will be limited to about 100 participants.

A flyer describing the Conference is available from:

Professor Mary Anne White
Chair, Gordon Research Conference on Order/Disorder in Solids
Department of Chemistry
Dalhousie University
Halifax, Nova Scotia
Canada B3H 4J3
Tel: 902-494-3894
FAX: 902-494-1310
Bitnet: MAWHITE@AC.DAL.CA

LIBRA

NMR Data Acquisition System



Imaging, Spectroscopy & Solid State Applications

tecmag

6006 Bellaire Blvd.
HOUSTON, TX 77081
Tel.: (713) 667-1507
Fax: (713) 667-3180

The **LIBRA** is the workhorse of the Zodiac Series. Numerous options are available to meet the needs of any NMR experiment. The LIBRA is conveniently packaged in a 7U 19" enclosure that is compatible with standard electronic racks. The basic hardware includes:

Pulse Programmer: LPUL

The pulse programmer has been specifically designed for Magnetic Resonance applications. It generates the different intervals required in NMR experiments, with 76 user defined output lines to control any device attached to it. This includes (but is not limited to) observe and multiple decoupler channels (RF gates, frequency, amplitude and phase), the magnetic field gradients in an Imaging or Gradient Enhanced Spectroscopy experiment, and the complete control of the signal averager. With a resolution and minimum pulse width of 100 ns, the pulse programmer has 5 independent 16-bit loop counters and a memory of 2 k x 128 bits. It allows the generation of any conceivable NMR sequence. The timing is controlled either by its own internal clock or by an external 10 MHz clock; the master clock of the spectrometer can be used for this purpose, providing perfect synchronization of the various units in the instrument. The pulse programmer is interfaced to the Macintosh II computer via a 32-bit parallel I/O board plugged into the NuBus. This interface board is included as part of the LIBRA system.

Signal Averager: LSA

Although digitizer boards from other manufacturers are available for the Macintosh II, the LIBRA signal averager is the only one which allows signal averaging. The signal averager is capable of acquiring data at a rate of up to 100 ns per complex point (2 channels), depending upon the speed of the Analog-to-Digital Converter. The LSA has 128 k x 32 bits of memory. The LSA comes in different versions:

- the - **S12**: 12-bit, 2.0 μ s/complex point (500 kHz bandwidth).
- the - **S16**: 16-bit, 3.5 μ s/complex point (285 kHz bandwidth).
- the - **F12**: 12-bit, 1.0 μ s/complex point (1 MHz bandwidth).
- the - **FTR**: 12-bit 5 MHz (10 MHz option) Transient Recorder with 8k x 16 bit memory.
- the - **LTRI**: transient Recorder interface for Nicolet Explorer or Biomation Units.

For other versions, please contact the factory.

Slow IO Interface Board: SIO

The Slow Input-Output Interface Board controls all non real time operations such as setting the spectrometer frequency, decoupler frequency, Bessel and/or Butterworth filter settings, the VT controller, etc. A 12-bit general purpose register is also provided. This register is used by the Spectrometer Module to control various spectrometer functions.

Spectrometer Module

Combined with the SIO board, the Spectrometer Module emulates all output lines of a commercial spectrometer (Bruker, Chemagnetics, GE/Nicolet, Jeol and Varian). These modules minimize interfacing problems.



Lilly Research Laboratories

A Division of Eli Lilly and Company

Lilly Corporate Center
Indianapolis, Indiana 46285
(317) 276-2000

July 21, 1993 (received 9/7/93)

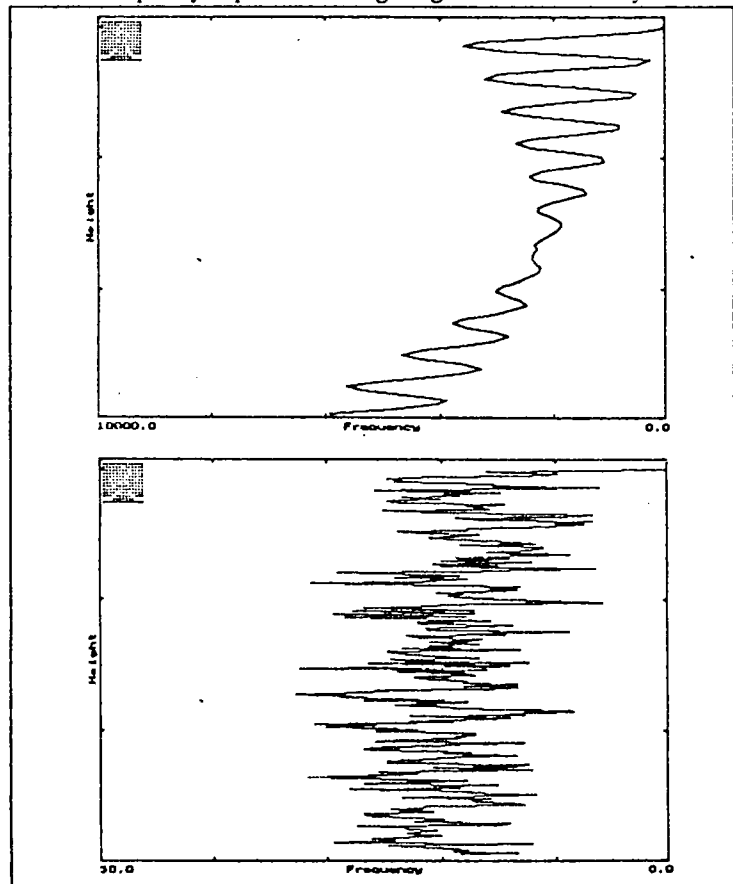
Dr. Bernard Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

A Step Towards Ultrahigh Resolution Proton NMR Spectroscopy

Dear Dr. Shapiro,

Several years ago, Professor Adam Allerhand and co-workers published a series of papers describing the development and applications of ultrahigh resolution carbon-13 and phosphorous-31 NMR spectroscopy.¹ Recently we have initiated a program to explore the possibilities, problems, and applications associated with ultrahigh resolution proton NMR spectroscopy. The goal of this program is to provide a quantum leap in the proton performance of current NMR instruments, and we would like to share with you some of our initial progress.

The first step in our program involved the installation and initial testing of a Resonance Research matrix shim system on a Varian Unity 300 spectrometer equipped with a Cryomagnet Systems probe. The Resonance Research matrix shim system (MHU-463) is a state-of-the-art magnetic field homogeneity adjustment coil system for solenoidal high-field NMR-quality superconducting magnets. This shim system is capable of correction up to 10th order axial and



6th order radial gradients, and utilizes fully digital, ultrastable current sources. Installation involved replacing the room temperature shim tube and the upper barrel with the MHU-463 shim tube and a Varian "500-style" upper barrel. Next, the 39 gradients produced by the MHU-463 were calibrated and purified using a helical magnetic field mapping procedure. The nominal magnetic field was mapped and analyzed into its component gradients from which an initial estimate for the magnitudes of the room temperature shim gradients was made. This process of mapping, analysis, and adjusting the shim gradients was conducted in automated cycles until the magnetic field homogeneity converged to a field of appropriate quality. The Figure to the left represents the projection of the helical path onto the axial translation axis covering ± 15 mm from probe center on a 7 mm radius for the unconverged (top) and converged (bottom) fields. As you can see from these plots, the field homogeneity over this region shows a significant improvement following convergence, and the converged field has a spread of only about 25 Hz over most of this region.

Figure 2

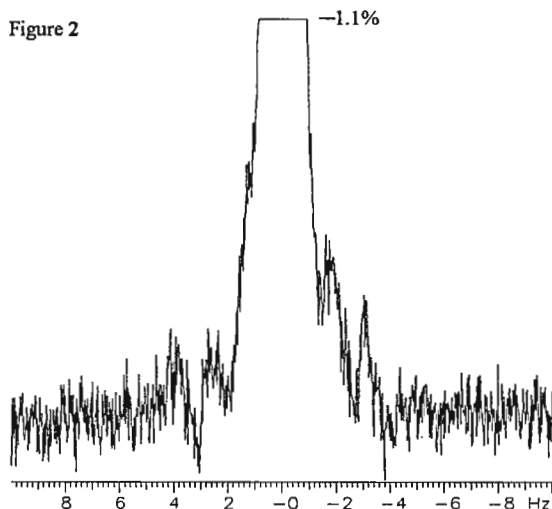


Figure 3

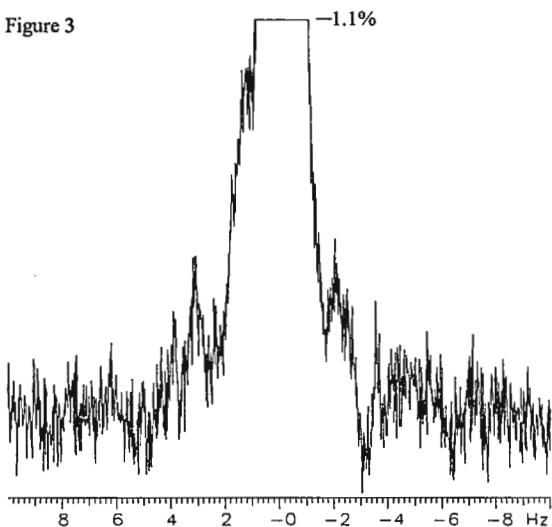
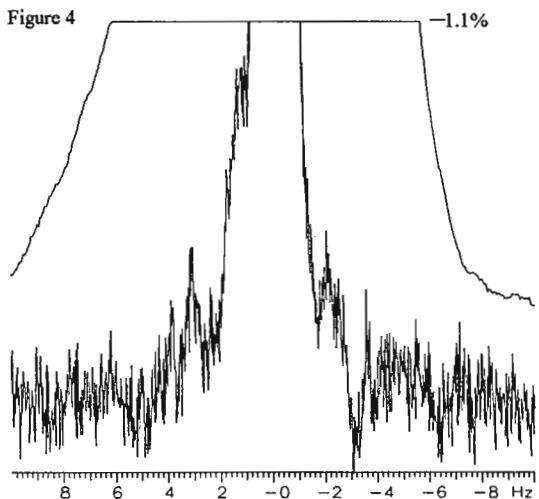


Figure 4



The bigger question is how does all this translate into performance? At the start of this project we identified several parameters with which to evaluate our progress including lineshape, resolution, sensitivity, system stability, reproducibility, and noise. Our best chloroform spinning and non-spinning lineshapes obtained using the standard Varian room temperature serial shim set and a Cryomagnet 5-mm probe after extensive shimming at 0.55% and 0.11% of full peak height were 3.5 Hz and 7.0 Hz, and 16 Hz and 29 Hz, respectively. Following conversion to the matrix shim system and shimming for about 2 hours starting from the converged open bore values, the spinning (Figure 2) and non-spinning (Figure 3) linewidths at 0.55% and 0.11% were 2.7 Hz and 4.3 Hz, and 3 Hz and 6 Hz, respectively. These results show a tremendous decrease in the non-spinning linewidths as would be expected when the radial gradients are correctly compensated and when the axial gradients are corrected to a high order. Practically speaking, we observe no difference between spinning and non-spinning lineshape performance. To better illustrate the magnitude of this improvement, Figure 4 shows a before (standard shim set) and after (matrix shim set) comparison of the non-spinning chloroform lineshape. We have also observed improvements in lock sensitivity and system stability. While these results are only preliminary, we are very encouraged by them and hope to report again soon on further developments.

Please credit this contribution to Doug Dorman's account.

Steve Maple

Steven R. Maple, Ph.D.
Pharmaceutical and Analytical Chemistry
Eli Lilly and Company


Piotr M. Starewicz

Piotr M. Starewicz, Ph.D.
Resonance Research

David Hillenbrand

David Hillenbrand, Ph.D.
Resonance Research

¹ S. R. Maple; J. E. Carson; A. Allerhand, *J. Am. Chem. Soc.* **1989**, *111*, 7293-7295, and references contained therein.



Magnetic Field Homogeneity Control Matrix Shim Systems

MHU-463/51: MHU-443/89

MHU-303/51: MHU-283/89

RESONANCE RESEARCH offers a broad range of state-of-the-art magnetic field homogeneity adjustment systems for solenoidal high-field NMR-quality superconducting magnets. These new designs offer performance unmatched by any existing shim system.

FEATURES:

- Unmatched homogeneity volume to bore size ratio
- Industry standard shim tube dimensions for 51, 54, and 89 mm magnets
- Axial and radial multi-coil design
- Axial correction capability to 8th order
- Radial correction capability to 6th order
- Powered from a fully digital, ultrastable current source
- Real-time Zo lock input (analog)
- Real-time homospoil input (TTL) trigger
- Staging by magnetic field mapping and analysis
- Gradient purification capability



RESONANCE RESEARCH

For 51 and 54 mm bore systems . . .

The MHU-463/51 system is *the* high performance magnetic field homogeneity adjustment coil system for high field NMR-quality superconducting magnets with a 51 or 54 mm bore. This system is capable of controlling up to 8th order axial and 6th order radial terms with substantial efficiency and without the loss of nominal bore dimensions.

The matrix shim system is based on an array of 48 magnetic coils which generate 39 gradients. Each coil is powered by an independent digitally controlled source under computer control. The operation of the shim system depends on the precise and simultaneous delivery of current to each coil in the array.

The MHU-303/51 system is designed for situations where appropriate control of the magnet can be effected by controlling fewer radial terms (while controlling the same number of axial terms). The system controls 32 coils which generate 27 gradients.

For a detailed description of Field Homogeneity in terms of the gradients described above, please request a copy of our technical report on Field Mapping Theory (Report Number 7/89)

MODEL	MHU-463/51	MHU-303/51
Gradient	$^1\text{H Hz/cm}^n$	$^1\text{H Hz/cm}^n$
z0	7500	7500
z	10000	10000
z2	1250	1250
z3	4000	4000
z4	750	750
z5	75	75
z6	100	100
z7	10	10
z8	5	5
x/y	3250	2000
zx/zy	2500	1250
c2/s2	1500	850
z2x/z2y	1500	800
zc2/zs2	1250	800
c3/s3	400	350
z3x/z3y	1000	750
z2c2/z2s2	1000	600
zc3/z3y	600	350
z4x/z4y	750	
z3c2/z3s2	750	
z2c3/z2s3	500	
z5x/z5y	250	
z4c2/z4s2	500	
z3c3/z3s3	250	

ACTIVE PARAMETERS

Field strengths indicated in the tables are specified for individual gradients within the family; in situations where several gradients within a family must be run at high values, it is possible that the maximum fields will not be achievable.

The specified values assume operation within the normal range of currents and are therefore conservative. Substantially higher individual gradients are achievable within the design, if required.

Additional adjustable gradients are implicit in the design but are not specified.

For 89 mm bore systems . . .

The MHU-443/89 system is *the* highest performance magnetic field homogeneity adjustment coil system for high field NMR-quality superconducting magnets with an 89 mm bore. This system is capable of controlling up to 7th order axial and 6th order radial terms with substantial efficiency and without the loss of nominal bore dimensions.

The matrix shim system is based on an array of 46 magnetic coils which generate 38 gradients. Each coil is powered by an independent digitally controlled source under computer control. The operation of the shim system depends on the precise and simultaneous delivery of current to each coil in the array.

The MHU-283/89 system is designed for situations where appropriate control of the magnet can be effected by controlling fewer radial terms (while controlling the same number of axial terms). The system controls 30 coils which generate 26 gradients.

MODEL	MHU-443/89	MHU-283/89
Gradient	$^1\text{H Hz/cm}^n$	$^1\text{H Hz/cm}^n$
z0	7500	7500
z	10000	10000
z2	750	750
z3	250	250
z4	25	25
z5	5	5
z6	2	2
z7	1	1
x/y	1250	1000
zx/zy	750	750
c2/s2	325	300
z2x/z2y	375	325
zc2/zs2	375	325
c3/s3	100	75
z3x/z3y	50	35
z2c2/z2s2	200	175
zc3/zs3	50	35
z4x/z4y	35	
z3c2/z3s2	25	
z2c3/z2s3	30	
z5x/z5y	3	
z4c2/z4s2	20	
z3c3/z3s3	10	

MECHANICAL SPECIFICATIONS

(typical configurations)

Magnet System	51/54 mm	89 mm
Outside Diameter	51.2 mm	88.25 mm
Inside Diameter (Shim)	40.1 mm	73.25 mm
Field Center to top of tube	86 mm	173 mm
Mounting Hole Pattern	95.25 mm	158.75 mm
	2 x M5	2 x M5
Base Thickness	25 mm	25 mm
Cable	6 m	6 m
Cooling	Forced air flow path provided	

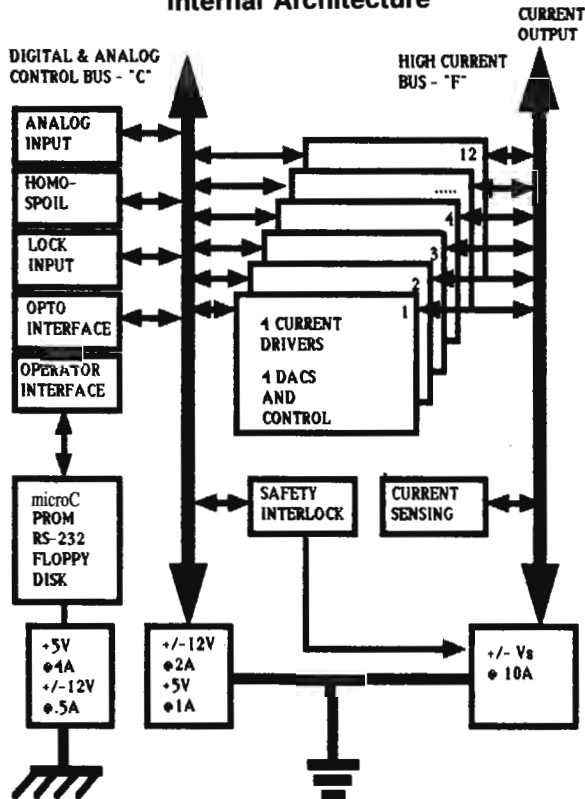
Please contact Resonance Research for special designs and special configurations.

A high stability power supply...

RESONANCE RESEARCH has developed an extremely high precision power supply to provide magnetic field stability.

The power supply for the magnetic homogeneity control system features high thermal stability (± 10 ppm FSR/degree) and temporal stability (± 5 ppm/day) to ensure that the magnetic correction is held constant. Various options can be provided including a direct Z_0 input and digital or direct analog input for the Homospoil function.

MHU-P Precision Current Sources Internal Architecture



Performance Specifications

Real time adjustment of gradient field strengths

Magnet drift compensation (linear ramp) up to 100 Hz/he.

Dynamic range in excess of 20 bits

22 bit resolution

Repeatability ± 5 ppm

True 16 bit monotonicity

Selectable current ranges from ± 20 mA to ± 4000 mA FSR

Setting time: better than 10 ms to 0.01% FSR

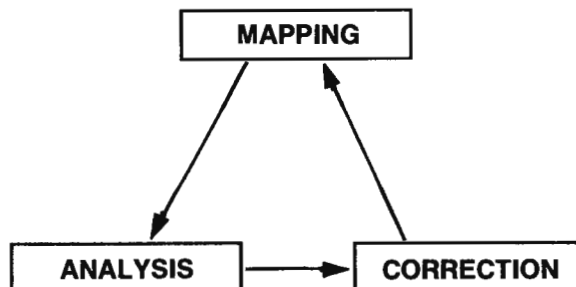
Staging and installation...

RESONANCE RESEARCH uses a state of the art, computer controlled, proton NMR based mapping system for the analysis of inhomogeneities and for shimming of superconducting magnets.

The mapping system is equipped with a helical-path electro-mechanical probe which acquires data suitable for simultaneous axial and radial analyses. The system completes a full mapping and analysis cycle in less than 40 minutes.

The ability of the mapping system to drive the shim power supply allows for very efficient magnet and shim staging. Detailed characterization and adjustment of room temperature shims in a fully automated map-analyze-shim cycles allows for optimum installation of the complex matrix shim system in less than 48 hours.

An iterative process to ensure homogeneity



For more information contact:

Resonance Research
43 Manning Rd.
Billerica, MA 01821
Tel (508) 671-0811
Fax (508) 663-0483

in the Western US

GMW
Box 2578
Redwood City, CA 94064
Tel (415) 368-4884
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HARVARD MEDICAL SCHOOL
DEPARTMENT OF BIOLOGICAL CHEMISTRY
AND MOLECULAR PHARMACOLOGY

Gerhard Wagner
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Fax (617) 738 0516

9/15/1993

(received 9/18/93)

Dear Barry:

In our ongoing exploration of the possibilities of Maximum Entropy reconstructions we are currently applying non-linear sampling to constant time experiments. While in usual non-linear sampling schemes the sampling schedule is dictated by the relaxation properties of the molecule, the choice is unconstrained in constant time experiments. Thus we searched for a sample schedule that minimizes artifacts and found that "random sampling" is the way to go.

Figure 1 shows a comparison between a ct-HCACO of the SH2 domain (Src-homology2) from protein tyrosine kinase p53^{Lck} processed in a conventional manner and the MaxEnt reconstruction of data where 10 points were randomly sampled out of 23 in the original dataset. The reconstruction was performed using the Rowland NMR Toolkit. The original data were extended by linear prediction prior to conventional processing but the dataset reconstructed with MaxEnt, though corresponding to less than 50% of the measuring time, has the same number of signals and a slightly better resolution.

Our experience shows, however, that the gain offered by this method should be invested in recording better spectra in the same amount of time rather than the same (wretched) quality in less time. Details will be published in the near future.

With best regards

Peter Schmieder
Peter Schmieder

Jeff Hoch
Jeff Hoch

Gerhard Wagner
Gerhard Wagner

Alan Stern
Alan Stern

Jonathan Lee
Jonathan Lee

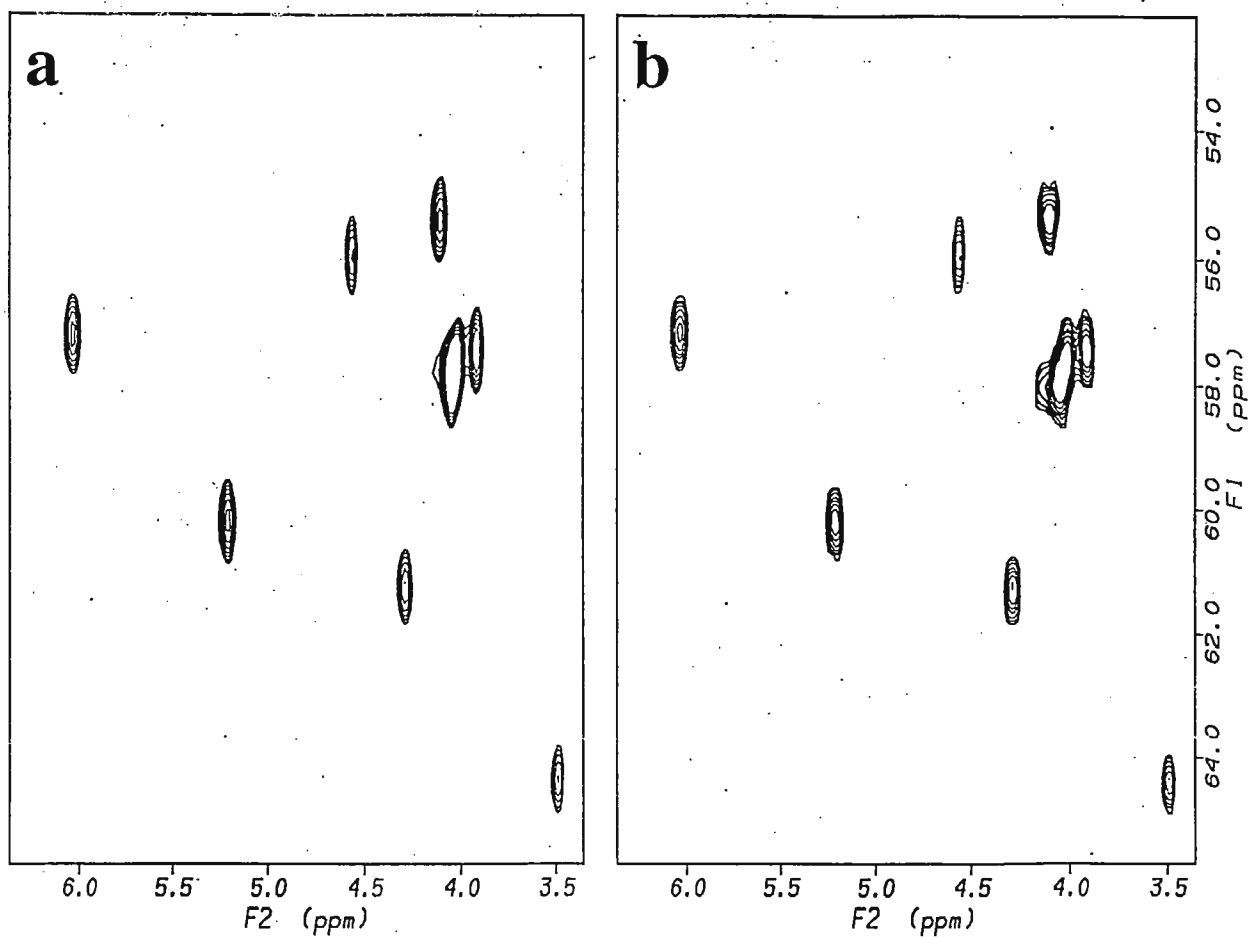


Figure 1. Comparison of 2D slices of a ct-HCACO recorded on a Varian Unity 500. (a) Processing with an DFT of 23 complex points extended to 32 by linear prediction (b) MaxEnt reconstruction of 10 points randomly selected out of the original 23.



Canada T6G 2G2

September 15, 1993

(received 9/20/93)

E3-44 Chemistry Bldg., Tel. (403) 492-3254 Fax (403) 492-8231

Dr. B.L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
PALO ALTO, CA, USA, 94393

Re: Artifacts generated by selective excitation

Dear Barry:

Recently we performed some 1D roesy experiments (1) on our Unity 500 to determine the conformation of a modified dinucleotide whose structure is shown below. The 1D roesy pulse sequence used was a shaped selective 90° pulse (a tophat 64 (2) of 146 ms duration) followed by a 90° purging pulse and a spin-lock period bracketted by 90° off-resonance compensation pulses then acquisition. When the frequency of the selective pulse was centered to excite the methylene protons (4.63 ppm) next to the CF_3 group, spectrum A was generated which shows a distorted multiplet for the strongly coupled H-5',5'' protons of both sugars. Initially we believed the observed "roesy" enhancement was distorted due to second order effects - a real noc to H-5' then a cross over to H-5'' via strong coupling. On further examination, the distorted multiplet was due to the sideband excitation of the H-5',5'' resonances due to pulse imperfections generated by the tophat 64 selective pulse (2). One can easily calculate the position of the sidebands by dividing the number of discrete steps (64) in the selective pulse by its total width (146 ms).

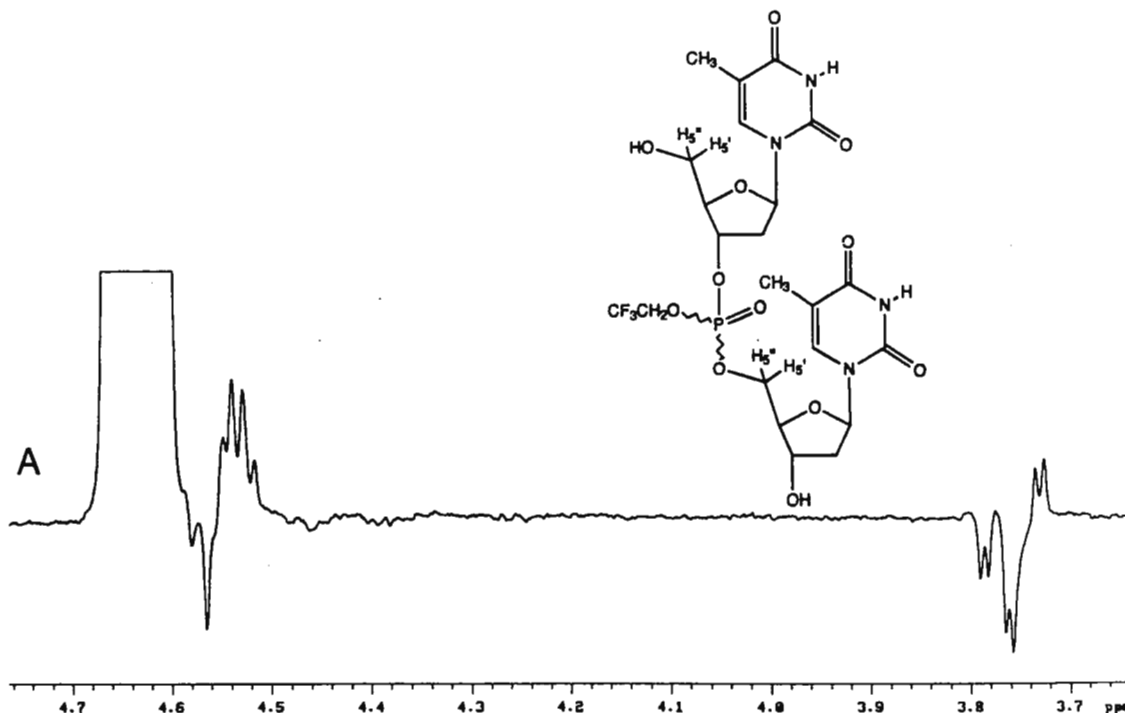
Sincerely,

Tom Nakashima

Tom

Nancy Fregeau - LeBlond
Nancy Fregeau

- 1) H. Kessler, U. Anders, G. Gemmecker, and S. Steuarnagel, *J. Magn. Reson.*, **85**, 1 (1989).
- 2) H. Geen and R. Freeman, *J. Magn. Reson.*, **93**, 93 (1991).





THE UNIVERSITY of SYDNEY
 DEPARTMENT of BIOCHEMISTRY
 SYDNEY, NSW 2006, AUSTRALIA

Telephone: (612)-692-4120
FAX: (612)-692-4726
E-mail: ismar-95@biochem.su.oz.au

Secretary: Dr Bill Bubb

4 February, 1993

Professor B.L. Shapiro
 966 Elsinore Court
 Palo Alto, CA 94303

Dear Professor Shapiro,

ISMAR 1995 in SYDNEY

The International Society of Magnetic Resonance will hold its 1995 conference in Sydney, Australia at the University of Sydney from 16-21 July, 1995. The conference will incorporate the biennial Australian Magnetic Resonance meeting and commemorate the 50th anniversary of the discovery of NMR.

The conference will provide an extensive scientific program in Australia's number one tourist destination. Sydney also offers accommodation to cater for all budgets and good international and domestic transport connections. Further details may be obtained from Dr. Les Field, Chair ISMAR-95 (E-mail: ismar-95@biochem.su.oz.au).

Yours sincerely,

Bill Bubb

For the ISMAR-95 Committee:

Les Field, Chair
 Dept of Organic Chemistry
 University of Sydney
 Sydney
 NSW 2006
 Australia
Fax: (612)-692-3329
Phone: (612)-692-2060

David Doddrell, Convenor
 Center for Magnetic Resonance
 University of Queensland
 St. Lucia
 QLD 4072
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 CSIRO
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 (612)-887-8489

Peter Barron

Michael Batley

Graham Bowden

Paul Callaghan

Bruce Cornell

John Hanna

Garry King

Glenn King

Philip Kuchel

Bridget Mabbutt

George Mendz

Barbara Messerle

Carolyn Mountford

Jim Pope

Graham Town

September 7, 1993 (received 9/11/93)

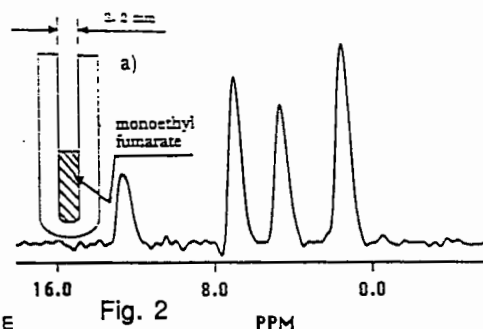
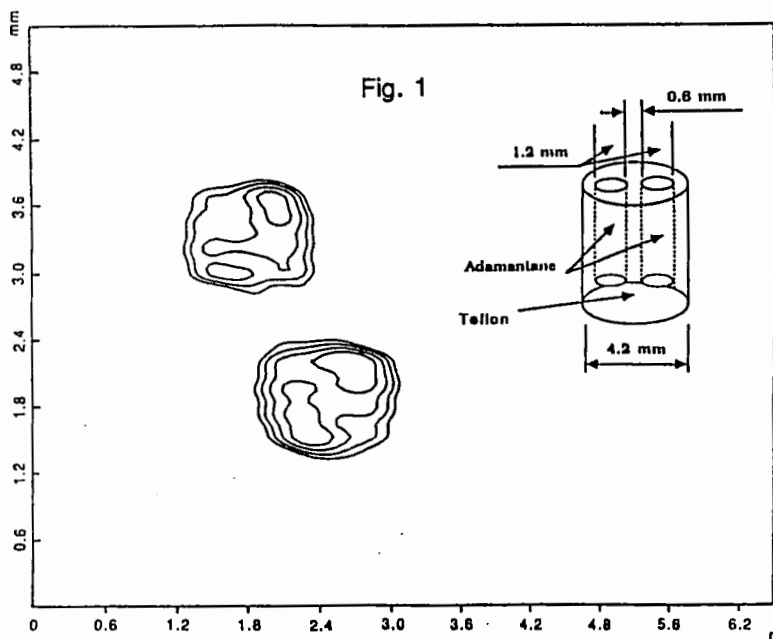
^1H CRAMPS Imaging of Solids; Old Nicolet Hardware

Dr. B.L. Shapiro
TAMU NMR Newsletter
966 Elsinore Ct.
Palo Alto, CA 94303

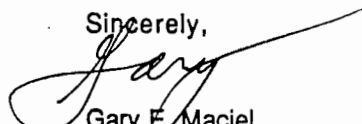
Department of Chemistry
Fort Collins, CO 80523
Tel: (303) 491-6480
Fax: (303) 491-1801

Dear Barry:

Although most of our current emphasis in MAS NMR imaging of solid samples is based on ^{13}C , much of our recent solid-sample imaging has been based on proton resonances. Our recent ^1H NMR imaging has utilized synchronized rotating gradients (as proposed by Wind and Yannoni and implemented by Cory, Reichwein, Vas Os and Veeman), together with TREV or BR-24 multiple-pulse line narrowing, MAS and *a pulse mode for the gradients*. This most recent ^1H CRAMPS imaging (carried out mainly by Yahong Sun and Jincheng Xiong) has involved both "soft" solids and "hard" solids. Figure 1 shows a 2-D transverse-plane spatial-spatial image (contour plot) of a phantom containing cylinders of adamantane. Figure 2 shows a 1-D spatial(transverse)-spectral image of a phantom containing a cylinder of monoethyl fumarate, a "hard" solid for ^1H CRAMPS. Above the spectral dimension is the ^1H CRAMPS (BR-24) spectrum of this compound obtained in our home-built imaging probe; clearly, a useful level of ^1H chemical shift resolution is retained in this experiment.



We have two old spectrometers that use 15-17 year-old Nicolet 1180 data systems, and we are looking for temporary measures to keep these data systems alive until we can afford to replace them with modern equipment. On the premise that one laboratory's junk might be another lab's salvation, we wonder if anyone has any functional Diablo Series 30 disc drives (or, even better, a functional Nicolet 1280/293B,C system) that we could acquire (steal!). Any help will be greatly appreciated, especially by students who are fighting against unreasonable odds to keep very old equipment running.

Sincerely,

Gary E. Maciel
Professor



Technische Universität München Garching bei München

Garching, 13. August 1993

Dr. B. L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto
California 94303
USA

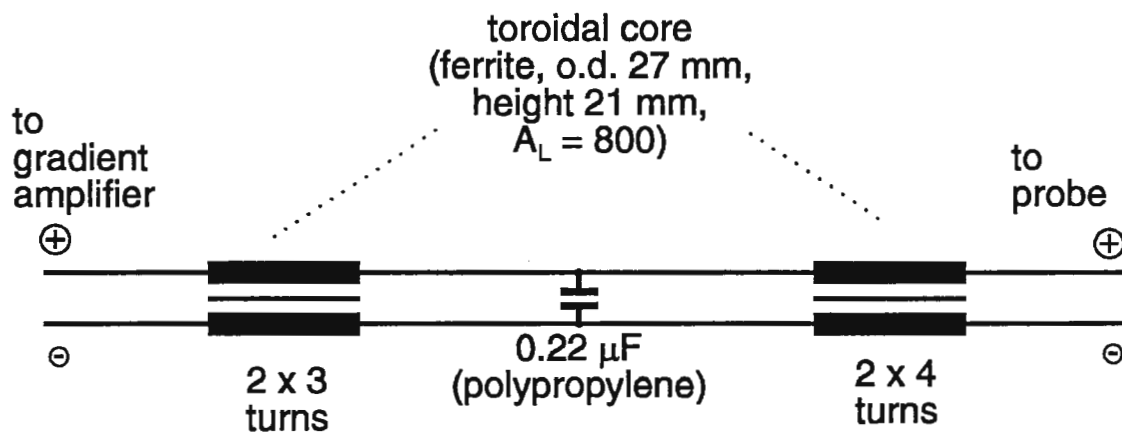
Dr. Rainer Haeßner
Organische Chemie II
AK Prof. Kessler
Lichtenbergstraße 4
D-85747 Garching

☎ (089) 3209-3300
Fax: (089) 3209-3210

(received 9/22/93)

Shielded Gradients with AMX600

Dear Dr. Shapiro,
we couldn't use the gradient unit of our Bruker AMX 600 spectrometer effectively due to a unique mistake. Each ^{15}N -pulse was picked up by the gradient coils with high amplitude (up to 40 V_{pp}). This signal arrived at the output of the gradient amplifier and caused the production of a gradient signal by this amplifier without any command to do this. Due to this effect it was impossible to detect any FID in the case of ^{15}N -CPD-decoupling. Attempts to repair the probe failed, so we decided to introduce a lowpass filter between probe and gradient amplifier. The electric scheme is given below.



All wires consist of copper with a diameter of 1.4 mm. The "plus" and "minus" wires on each core are wound in opposite direction, respectively. The effect on the gradient preemphasis was quite small und could be readjusted easily.

Please credit this contribution to Prof. Köhler's account.

Sincerely,

Rainer Haeßner

Gerd Gemmecker

TAMU NMR Newsletter

Policies and Practical Considerations

(Slightly Revised October 1993)

The TAMU NMR Newsletter (formerly the IIT NMR Newsletter, and originally the Mellon Institute NMR Newsletter) continues with the same name, under the aegis of Texas A&M University, although the undersigned Editor/Publisher now resides in California. The Newsletter, now beginning its thirty-sixth year of consecutive monthly publication, continues under the same general policies as in the past. All communication with the Newsletter must be directed to the address overleaf.

1. Policy:

The TAMU NMR Newsletter is a means for the rapid exchange of information among active workers in the field of NMR spectroscopy, as defined broadly, including imaging. As such, the Newsletter serves its purpose best if the participants impart whatever they feel will interest their colleagues, and inquire about whatever matters concern them.

Since the subscriber/participant clearly is the best judge of what he or she considers interesting, our first statement of policy is "We print anything." (This is followed by the reservation, "that won't land us in jail or bankruptcy court.") Virtually no editorial functions are performed, although on rare occasions there is the need to classify a contribution as 'not for credit'. I trust that the reasons for this policy are obvious.

The Newsletter is not, and will not become, a journal. We merely reproduce and disseminate exactly what is sent in. Foreign participants should not feel obliged to render their contributions in English.

2. Public Quotation and Referencing:

Public quotation of Newsletter contents in print or in a formal talk at a meeting, etc., is expressly forbidden (except as follows), and reference to the TAMU NMR Newsletter by name in the scientific literature is never permissible. *In order to quote results or use material from the Newsletter, it is necessary, in each individual case, to obtain the prior permission of the author in question and then to refer to the material quoted as a "Private Communication".* If your copy of the Newsletter is shared with other readers, it is your obligation as the actual recipient of the Newsletter to see that these other readers of your copy are acquainted with, and abide by, these statements of policy.

3. Participation is the prime requisite for receiving the TAMU NMR Newsletter: In order to receive the Newsletter, you must make at least occasional technical contributions to its contents.

We feel that we have to be quite rigorous in this regard, and the following schedule is in effect: Eight months after your last technical contribution, you will receive a "Reminder" notice. If no technical contribution is then forthcoming, ten months after your previous contribution you will receive an "Ultimatum" notice, and then the next issue will be your last, absent a technical contribution. Subscription fees are not refunded in such cases. If you are dropped from the mailing list, you can be reinstated by submitting a contribution, and you will receive back issues (as available) and forthcoming issues at the rate of nine per contribution.

Frequent contributions are encouraged, but no "advance credit" can be obtained for them. In cases of joint authorship, either contributor, but not both, may be credited. Please indicate to whose account credit should be given. Please note that meeting announcements, as well as "Position Available," "Equipment Wanted" (or "For Sale"), etc., notices are very welcome, but only on a not-for-credit basis, i.e., such items do not substitute for a *bona fide* technical contribution. Similar considerations must occasionally be applied to a few (quasi-)technical items.

4. **Finances:** The Newsletter is wholly self-supporting, and its funding depends on Advertising, Sponsorships, and individual Subscriptions. The Subscription fee for the October 1993 - September 1994 year remains US\$170.00, with a 50% academic or personal subscription discount. Subscriptions are available only for the twelve monthly issues which begin with the October issue and run through that of the following September. However, a subscription can be initiated at any time, and the issues back to the previous October will be provided as long as copies remain available.

Corporations are also invited to consider joining the list of Sponsors of the Newsletter. Sponsors' names appear in each month's Newsletter, and copies of the Newsletter are provided to all Sponsors. The continuation of this non-commercial Newsletter depends significantly on the interest and generosity of our Sponsors, most of whom have been loyal supporters of this publication for many years. We will be happy to provide further details to anyone interested.

Continued

Another major, indeed most essential, source of funds for the Newsletter is Advertising. We earnestly encourage present and potential participants of the Newsletter to seek advertising from their companies. Our rates are very modest - please inquire for details.

5. Practical Considerations:

- a) All technical contributions to the TAMU NMR Newsletter will always be included in the next issue if received before the published deadline dates.
- b) Please provide short titles of all topics of your contributions, so as to ensure accuracy in the Table of Contents.
- c) Contributions should be on the *minimum* (NOTE!!) number of 8.5 x 11" (21 x 27.5 cm) pages, printed on one side only. Contributions may not exceed three pages without prior approval. Each page must have margins of at least 0.5 - 0.75" (1.3 - 2.0 cm) on all sides. Please observe these limits. Black ink for typing, drawings, etc., is essential. All drawings, figures, etc., should be mounted in place on the 8.5 x 11" pages. We are not equipped to handle pieces of paper larger than 8.5 x 11" (21 x 27.5 cm).

Please do not fold, clip, or staple your pages. Protect the condition of your letters from the ravages of the mails by enclosing what you send in a cardboard or plastic folder, etc.

Foreign subscribers are reminded that regardless of the standard paper length you use, all material - letterhead, text, figures, addresses printed at the page bottom, everything - must not exceed 10" (ca. 25.3 cm) from top to bottom.

Significant savings of Newsletter pages and total space can be made by exercising close control over the formatting and type sizes of the contributions. Please consider the following:

i) For those with computers, try using a smaller type font. The body of this page is printed in 11 point type, which I believe is adequate for most purposes. Even 12 point is acceptable, I suppose. Those who are computerized can also employ non-integral spacing of lines so that sub- and superscripts don't collide with lines below and above.

ii) **PLEASE avoid excessive margins.** *Instruct your secretaries to avoid normal correspondence esthetics or practices, however time-honored or 'standard'!* This page has margins on both sides of 0.6" (ca. 1.55 cm), which is very adequate. Margins of the same size at the top and bottom are sufficient also, but don't worry if there is more space at the end of your document, for I can often use such spaces for notices, etc.

Also, please avoid large amounts of unused space at the top of letters. Give thought to the sizes of figures, drawings, etc., and please mount these so as to use the minimum space on the page.

iii) 'Position Available', 'Equipment Wanted', and Similar Notices. These are always welcome, but not for subscription credit, of course. Such notices will appear, however, *only* if received with these necessarily rigid constraints: a) Single spaced; b) both side margins 0.6 - 0.7" (1.5 - 1.7 cm.)- NOT WIDER; c) the minimum total height, please, but definitely no more than 4.5" (11.5 cm.).

iv) **AVOID DOUBLE SPACING LIKE THE BLACK PLAGUE !!!** This is extremely wasteful of space. Even sans computer, small type and 1.5-line (if needed) spacing can be had with a little effort.

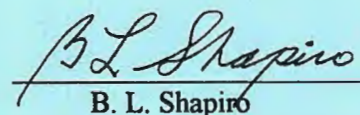
6. Suggestions: They are always welcome.

Address for all correspondence:

Dr. Bernard L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, California 94303
U.S.A.

Telephone: (415) 493-5971. Please confine telephone calls to the hours from 8:00AM - 10:00PM, *Pacific Coast Time*.

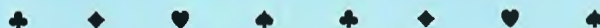
FAX: (415) 493-1348 (Do not use for technical contributions which are to appear in the Newsletter, for the quality is not adequate.)


B. L. Shapiro

1 October 1993

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All Newsletter correspondence should be addressed to

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(415) 493-5971 - Please call
only between 8:00 am and
10:00 pm, Pacific Coast time.

Deadline Dates

No. 423 (December)	19 November 1993
No. 424 (Jan. 1994)	17 December 1993
No. 425 (February)	21 January 1994
No. 426 (March)	18 February 1994



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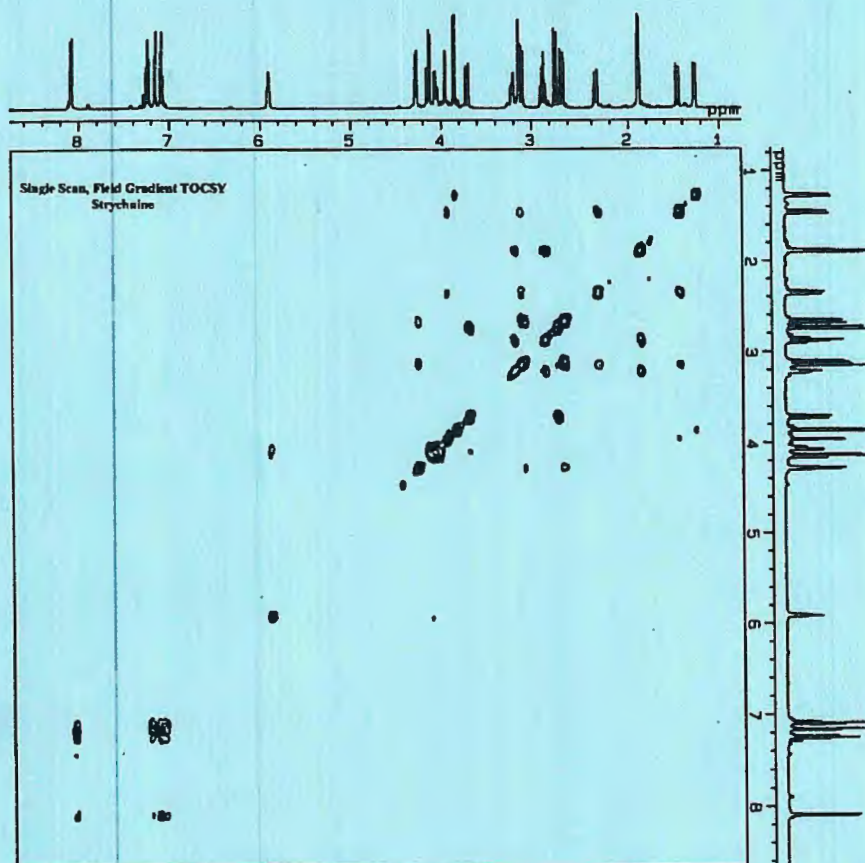
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If the mailing label on your envelope of this issue is adorned with a large red dot or circle: this decoration means that you will not be mailed any more issues until a technical contribution has been received by me.



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