TEXAS A&M UNIVERSITY

NMR NEWSLETTER

No. 428

May 1994

TABLE 1 DEUTERATED SOLVENTS

Cat. No.	Description	Formula	Min. Iso. (Deuterium)	Density (g/cc)	MP (°C)	BP (°C)	$-\chi_v \times 10^6$ @ (°C)
D-11	Acetone-d_6	CD_3COCD_3	99.5%	1.12	-97	56	0.551 (32)
D-120	Acetone-d_6 + 1% TMS		99.5%				
D-13	Acetone-d_6	CD_3COCD_3	99.8%	0.87	-94	57	0.460 (20)
D-121	Aceonte-d_6 + 1% TMS		99.8%				
D-129							
D-14							543 (20)
D-21							0 611
D-122							
D-130							
D-28	Chloroform-d	$CDCl_3$	99.8%	1.50	-64	62	0.740 (20)
D-31	Chloroform-d + 1% TMS		99.8%				

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Cat. No.	Size	Instrument Model	Type
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WCV-XL (XL-100)	11" X 26"	XL-100 (and FT)	Gridded-Two Color
WCV-XLFT-100	11" X 26"	XL-100 (and FT)	Gridded-Two Color
WCV-XL-200	11" X 26"	XL-200, XL-300, XL-400	Gridded-Two Color
WCV-20 (CFT-20)	11" X 16 3/4" X 17"	CFT-20, FT-80, FT-80A All Models	Gridded-Two Color Blank

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FORTHCOMING NMR MEETINGS

Gordon Conference on Magnetic Resonance in Biology and Medicine, New England College, Henniker, NH, **July 17 - 22, 1994**; Contact: Dr. Carlyle B. Storm, Director, Gordon Research Conferences, Gordon Research Center, Univ. of Rhode Island, Kingston, RI 02881-0801; Tel. (401) 783-4011 or -3372; Fax: (401) 783-7644.

8th International Symposium on Molecular Recognition and Inclusion, Ottawa, Ontario, Canada, **July 31 - August 5, 1994**; Contact: H. Morin-Dumais, Steacie Institute for Molecular Sciences, National Research Council of Canada, 100 Sussex Drive, Ottawa, ON K1A 0R6, Canada; (613) 993-1212; Fax: (613) 954-5242 See TAMU NMR Newsletter 427, 38

Solid-State NMR Symposium, 36th Rocky Mountain Conference on Analytical Spectroscopy, Denver, CO, **July 31 - August 5, 1994**; Contact: R. E. Botto, Chemistry Divn., Argonne Natl. Lab., Argonne, IL 60439; (708) 522-3524; Fax: (708) 252-92882 See TAMU NMR Newsletter 424, 46.

2nd Meeting, Society of Magnetic Resonance, San Francisco, California, **August 6 - 12, 1994**; Contact: SMR Berkeley Office, 1918 University Ave., Suite 3C, Berkeley, CA 94704; Tel. (510) 841-1899; Fax: (510) 841-2340.

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.

XVIth International Conference on Magnetic Resonance in Biological Systems, Veldhoven, The Netherlands, **August 14 - 19, 1994**; Organizing Committee: M. J. A. de Bie, C. W. Hilbers, R. Kaptein; Contact: Secretariat XVIth ICMRBS, Bijvoet Center for Biolmolecular Research, Padualaan 8, NL-3584 CH Utrecht, The Netherlands; Tel. +31 30 53 2652/2184/3801; Fax: +31 30 53 7623/54 0980.

Ampere Summer School on Magnetic Resonance with Spatial Resolution, Eichstätt, Bavaria, Germany, **September 2 - 8, 1994**; Contact: L. D. Hall or B. Blümich - See TAMU NMR Newsletter 426, 56.

FACSS XXI (21st Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies, St. Louis, Missouri, **October 2 - 7, 1994**; Held jointly with the MMRS-5 meeting *(v.i.)*. Contact: FACSS National Office, 198 Thomas Johnson Drive, Suite S-2, Frederick, MD 21702-4317; Phone: (301) 846-4797. See TAMU NMR Newsletter 428, 28.

5th Missouri Magnetic Resonance Symposium, St. Louis, Missouri, **October 5 - 6, 1994**; Held jointly with the FACSS meeting *(v.s.)*. Contact: FACSS Natl. Office, 198 Thomas Johnson Dr., Suite S-2, Frederick, MD 21702-4317; Phone: (301) 846-4797. See TAMU NMR Newsletter 428, 28.

Continued on page 38

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April 8, 1994
(received 4/18/94)

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

Merged Biomedical Magnetic Resonance Societies

Dear Barry:

I wish to bring to the attention of readers of this august journal a matter that has arisen as a result of the merger of the Society of Magnetic Resonance in Medicine and the Society for Magnetic Resonance Imaging.

These two well respected and influential international societies devoted to biomedical and clinical applications of magnetic resonance have, after some years of discussions, agreed to merge. In my opinion, this merger will produce a single more effective organization which can better serve its combined membership while reducing needless duplication.

However, I and many others both within and outside the biomedical research community are troubled by the name chosen for the new group, "Society of Magnetic Resonance." Despite the unambiguous focus on biomedical and clinical application and practice, this new name suggests that it is the primary society for magnetic resonance activities worldwide, and by implication that its journals are the primary sources for the magnetic resonance literature. It flies in the face of venerable institutions such as the ENC, EENC, Groupment Ampere, ISMAR, the Journal of Magnetic Resonance, and others.

As a result of some rather impassioned dissent by a number of member and nonmember scientists, a vote to change the name was recently held. Those members who voted did indeed favor a name change by 61.4 percent. However, the bylaws require a 2/3 majority for such a change, and so it did not pass.

Scientists, journal publishers, funding agencies, educational institutions, scientific societies and instrument vendors alike should be concerned that such things as organization names accurately reflect their intended missions and constituencies.

I urge you to express your views promptly (*i.e.*, well in advance of the August board meeting) to:

Dr. Stephen J. Reiderer, President
Society of Magnetic Resonance
1918 University Avenue, Suite 3C
Berkeley, CA 94704, USA
Fax: 001-510-841-2340

Best regards,

Jerry

Jerome L. Ackerman

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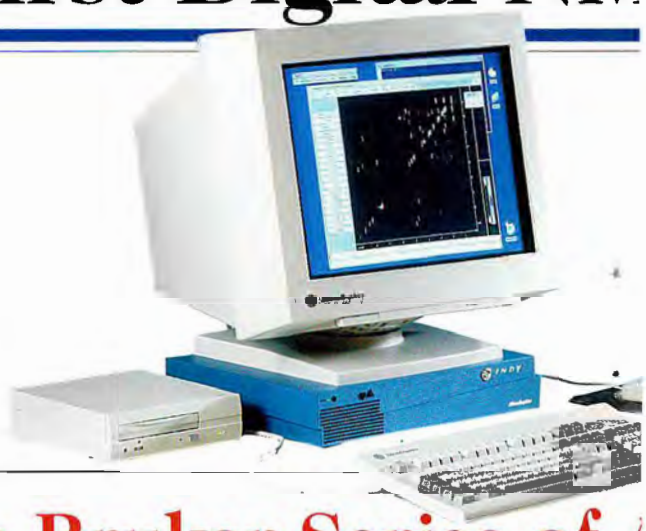

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DIGITAL FEATURES		
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Real time data decimation	Yes, via dedicated DSP processor	
Digital lock with real-time quadrature detection	Yes, via dedicated DSP processor	
Real-time gradient calculation	Yes, via dedicated DSP processor	
PROBES		
GRASP with Z-gradient	Yes	
GRASP with X, Y and Z-gradients	Yes	
RF GRASP	Yes	
2.5 mm micro-sample probes	Yes, including inverse triple resonance	
8 mm probes	Yes, including inverse triple resonance	
Quadra-nuclear inverse probes	Yes	
SOLIDS		
Pneumatic sample ejection	Yes	
Automatic sample changer	Yes	
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MARBURG, DEN 12. April 1994

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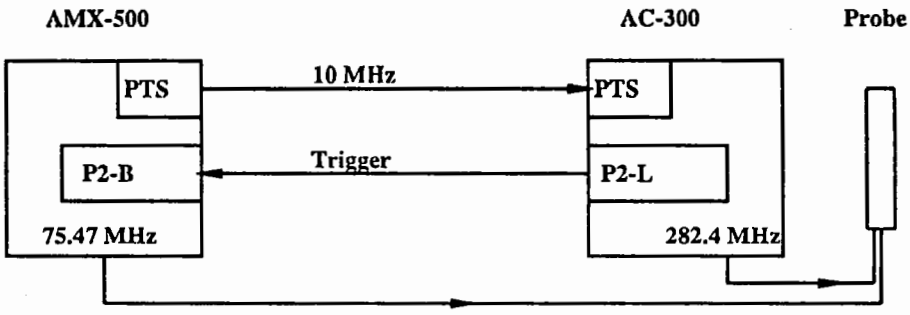
(received 4/20/94)

Prof. Dr. B. L. Shapiro
TAMU-NMR Newsletter
966 Elsinore Court
Palo Alto, CAL. 94303
USA

Two NMR Instruments Combined In One Experiment: $^{13}C,^{19}F$ Correlation

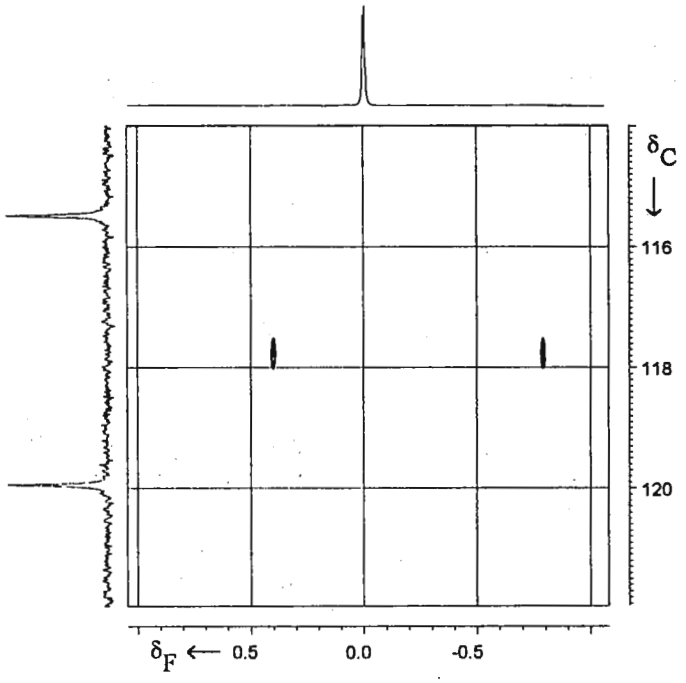
Dear Barry,

In our series of 2D $^{13}C,^{n}X$ correlation experiments [1-7] we had so far not looked at fluorine, although a $^{13}C,^{19}F$ correlation should be theoretically straightforward and chemically highly desirable both due to the 100% natural abundance and high sensitivity of fluorine and due to the wealth of polyfluorinated compounds. The reason for neglecting fluorine is an experimental one: To perform this kind of experiment one would need a special probe allowing for ^{13}C, ^{19}F and ^{1}H frequencies and an instrument which contains an independant third frequency channel operating at the fluorine frequency, surely a costly arrangement. To use the usual „inverse" mode of two channel spectrometers is not possible, since fluorine is handled as X-nucleus by most instruments.
Discussing the problem with Norbert Wetzel, our Bruker service engineer, he proposed a remarkable simple solution. Thus, in this letter we show, how a $^{13}C,^{19}F$ correlation can be performed *at no additional cost* provided one has a ^{19}F preamplifier and not just one, but two nmr instruments in possession. Choosing polyfluorinated compounds with no hydrogen atoms the experiment can be performed on a standard dual $^{13}C,^{1}H$ probehead, the ^{1}H coil being tuned to the fluorine frequency.



The fluorine frequency is generated on a Bruker AC-300 instrument, whereas the carbon pulses are drawn from a nearby AMX-500. Of course the instruments have to be synchronized. The 10 MHz PTS frequency of the AMX is used to drive the AC-300, the pulse program at the AC-300 uses the

external pulse option providing a trigger pulse (RCP 6 at process controller P2-L) to generate the carbon pulses on the AMX. The AMX receives the trigger pulses via its external trigger option at process controller P2-B. Thus a pulse program at the AMX waits for the corresponding trigger pulses from the AC-300 to send carbon RF pulses to the AC-300 probehead.
Of coarse we started with the most simple compound $CFCl_3$, the reference compound of ^{19}F NMR. In the fig. the 2D $^{13}C,^{19}F$ correlation spectrum is shown; note the large isotope effect of ^{13}C nuclei bound to ^{19}F. Chemically more demanding examples are currently being measured.



With all best wishes

Prof. Dr. S. Berger

Norbert Wetzel
(Bruker Karlsruhe)

[1] $^{13}C,^{11}B$: T. Fäcke, and S. Berger, *Magn. Reson. Chem.*, in press.
[2] $^{13}C,^{29}Si$: S. Berger, *J. Magn. Reson. Ser. A*, **101**, 329 (1993).
[3] $^{13}C,^{31}P$: P. Bast, S. Berger, and H. Günther, *Magn. Reson. Chem.*, **30**, 587 (1992).
[4] $^{13}C,^{77}Se$:T. Fäcke, R. Wagner, and S. Berger, *J. Org. Chem.*, **58**, 5475 (1993).
[5] $^{13}C,^{119}Sn$: S. Berger, and T. N. Mitchell, *Organometallics*, **11**, 3481 (1992).
[6] $^{13}C,^{199}Hg$: T. Fäcke, and S. Berger, *J. Organomet. Chem.*, in press.
[7] $^{13}C,^{207}Pb$: T. Fäcke, and S. Berger, *Main Group Metal Chem.*, in press.

University of Illinois
at Urbana-Champaign

School of Chemical Sciences
1209 West California Street
Urbana, IL 61801

(received 3/24/94)

Dear Dr. Shapiro,

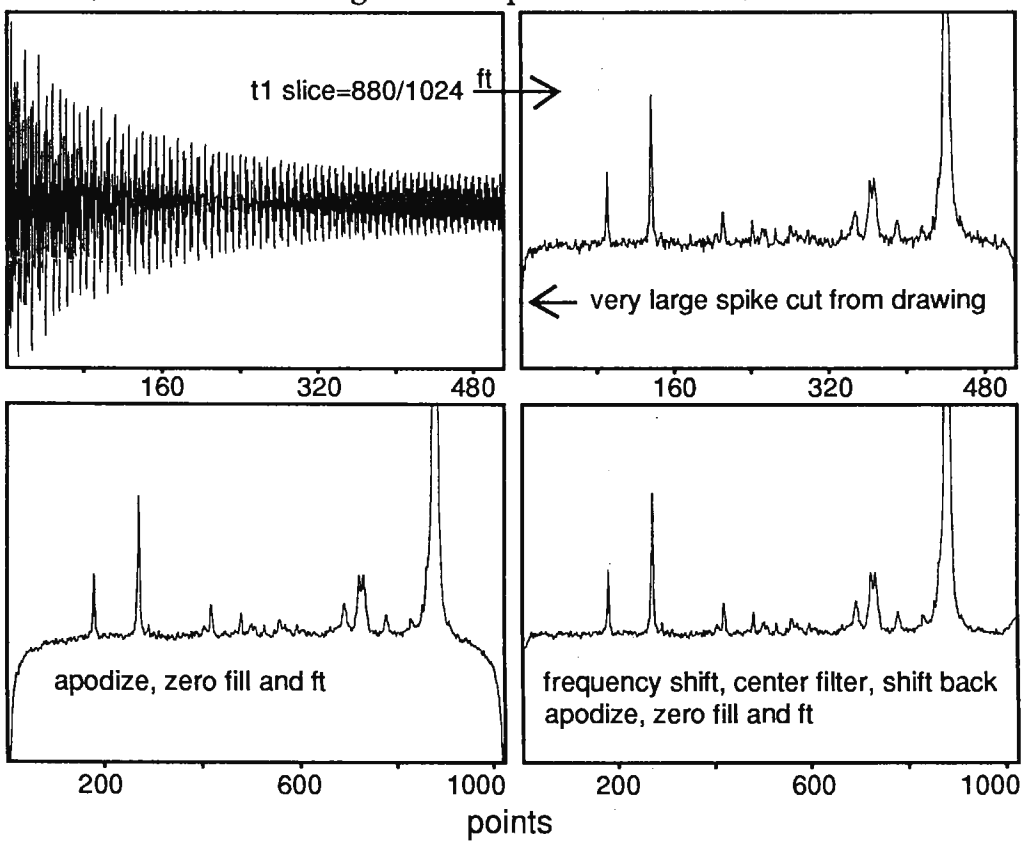
March 21, 1993

Frequency Shifting in the Time Domain

Our goal is to perform a 2D-NOESY in a minimum amount of machine time. This can be important in titrations where multiple 2D-NOESY's will be needed, and also for higher dimensional experiments where there are severe time constraints. There are two obvious aspects of the 2D-NOESY that can be addressed; first the relaxation delays can be reduced, and second, the need for phase cycling in the evolution dimension can be reduced.

We present here a 2D-NOESY that was collected in 30 minutes with conventional equipment (Varian VXR-500 spectrometer with Nalorac inverse detection probe) and processed with Felix (v.2.x or 1.1). Reductions in both the relaxation delay and t1 phase cycling were exploited. The relaxation delay, which started at 4 seconds, was progressively reduced as the t1 increased so that the effect on the signal was equivalent to 4 Hz exponential multiplication. This progressively reduced relaxation time shortened the accumulation time by one half (this technique will be described in detail elsewhere, and does not affect the frequency shifting).

The data was collected as 512 complex t1 increment blocks with 1024 complex points each. Only one scan was collected for each t1 increment. The TPPI-States phase cycle was applied in the t1 dimension so the artifacts, which mainly arise from relaxation in the mixing period, are placed at the edge of the spectrum. A t1 slice through a methyl group near the edge of the spectrum is shown in the upper left panel of the figure (this is the worst case). The artifacts cause large spikes at the edges of the frequency transformed spectrum (upper right). When apodization is added, these artifacts degrade the spectral baseline (lower left).



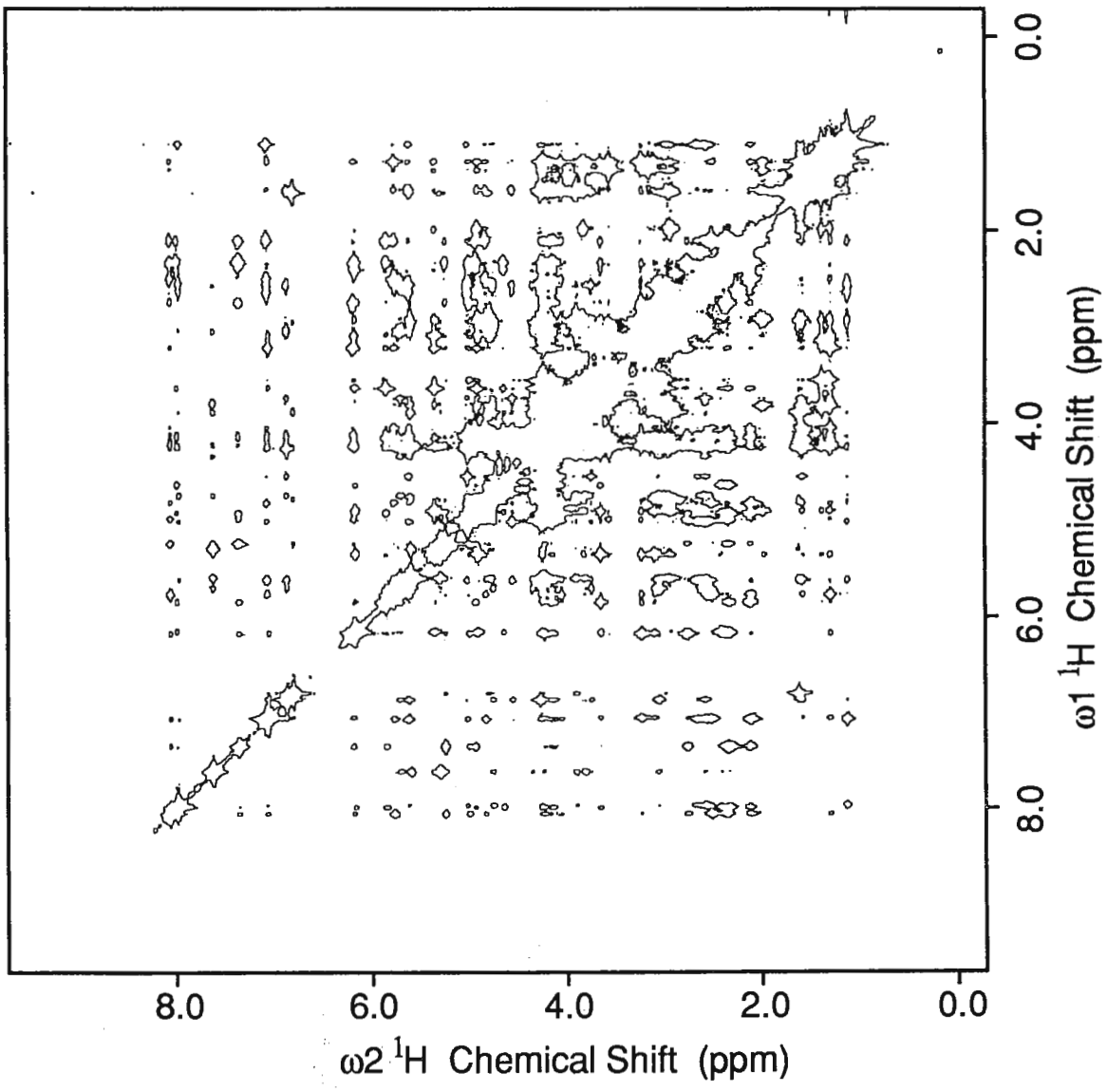
Removal of these artifacts must be performed before apodization. The artifact removal is performed by the time domain filter of Marion (J. Mag. Res., 84, 425, 1989) which subtracts a zero Hz notch from the real and imaginary t1 data separately. Since the phase increment is at exactly half the frequency of the data point collection, the artifacts we wish to remove are at the edges of the frequency spectrum. Thus, we shift the frequencies of the signals by half the spectral width using a simple procedure in Felix, as follows: first, generate a non-decaying FID with the frequency of the required shift (ze, gf 2500 1e6), second multiply the t1 slice with this FID. Next, apply the Marion filter (cnv 0 32), then reverse the frequency shift process. In this simple way the notch filter can remove any desired frequency. The resulting 30 minute 2D-NOESY is shown below where the contour is just above the noise level and no baseline correction is required.

Sincerely

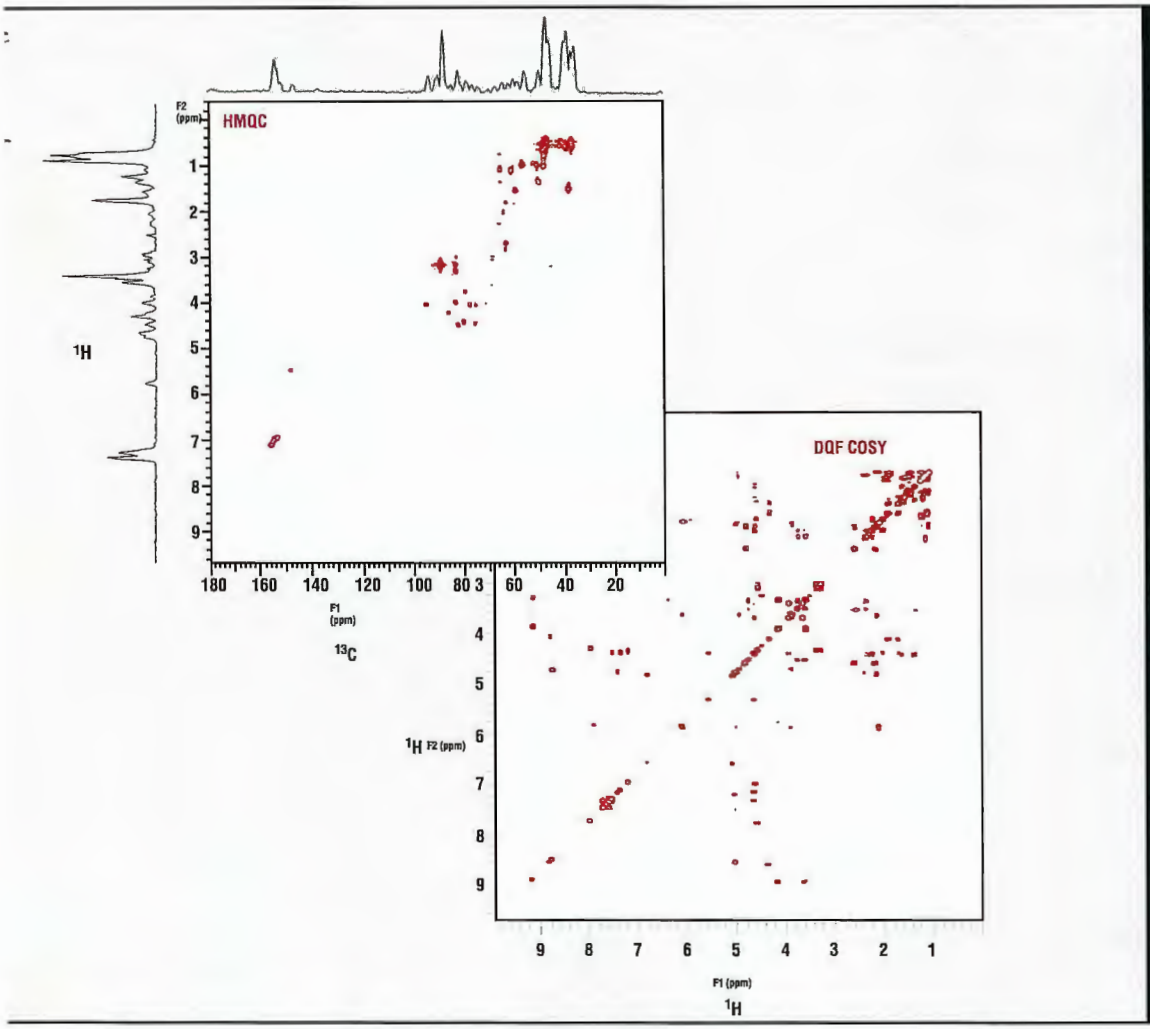
Zhehong Gan Howard Robinson

email: gan@aries.scs.uiuc.edu or hhr@uiuc.edu

credit to: Dr. Vera Mainz.



High-performance Pulsed Field Gradients



a) HMQC spectrum of peptide in DMSO-d_6, 2 transients per increment.

b) DQF COSY spectrum of peptide in DMSO-d_6, 1 transient per increment.

Both spectra were acquired using a UNITYplus 400 spectrometer, an Indirect•nmr Pulsed Field Gradient probe, and the Performa I Pulsed Field Gradient module.

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March 31, 1994
(received 4/8/94)

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

ANALYSIS OF ANOXIC FTBA RELAXATION DATA

Dear Barry,

To use the T_1 of ^{19}F of perfluorocarbon emulsions as an *in vivo* probe of tissue oxygenation, we need to know the T_1 value of the various NMR peaks over a range of temperatures at zero oxygen pressure at any reasonable Larmor frequency. We made extensive measurements at 7.05 tesla of the ^{19}F T_1 of the four resonance peaks of perfluorotributylamine (FTBA), $N[(CF_2)_3CF_3]_3$, over a temperature range that includes the T_1 minimum of the CF_2 resonances. To get an overall understanding of the relaxation, we made a simple interpretation, based on elementary relaxation theory, and were surprised at how well this approach models the data.

The pattern of the T_1 dependencies of the different resonances on temperature provides us with a guide to model the data. The observation of T_1 minima for the three CF_2 at approximately 270 °K allows us to estimate the correlation time τ_c that describes random molecular tumbling. However, we did not observe a T_1 minimum for the CF_3 peak. In addition, at temperatures above the CF_2 T_1 minimum, the CF_3 T_1 value is *greater* than the CF_2 values, even though the magnetic dipole-dipole (DD) interactions in a CF_3 group are twice as large as in a CF_2 group. These two observations may indicate that (1) the CF_3 groups are reorienting, inside the molecule, about their symmetry axis, and (2) that chemical shift anisotropy (CSA) is an important relaxation mechanism for FTBA. The reasoning is as follows: at temperatures above the T_1 minimum, internal motion reduces the $1/T_1$ contributions from both the DD and CSA interactions; the percentage reduction is greater for the CSA interaction than for the DD interaction because of the geometry of the CF_3 group and the different trigonometric dependencies of the DD and CSA interactions. Otherwise, if internal motion did not occur, the CF_3 resonance would have *smaller* T_1 values than the CF_2 resonances and would have a T_1 minimum at approximately the same temperature.

We estimate the relative contributions of the DD and CSA relaxation mechanisms by using the following assumptions to model the data: (1) all relaxation contributions arise within the CF_2 or CF_3 group, (2) both DD and CSA relaxation contributions contribute separately and additively to $1/T_1$, (3) the CF_2 groups are motionless and fixed in a rigid sphere that undergoes isotropic rotational diffusion, (4) τ_c of this rotational diffusion obeys the Arrhenius equation, (5) the CF_3 group undergoes random internal 120° jumps about the three-fold symmetry axis as described by the Arrhenius equation, (6) the CSA lies along the C-F bond, and (7) the CSA parameters for CF_2 fluorines are those for Teflon and those for the CF_3 fluorines are those for CF_3-COOAg.

First, we model the CF_2 relaxation by adjusting E_a, τ_c^0, and r_{FF} so that the computed T_1 versus temperature curve visually fits the data. We find that a single value of E_a and τ_c^0 describes all of the CF_2 data. Using these two values, we find r_{FF} for each CF_2 resonance:

E_a = 5.7 kcal/mole — r_{FF} (at -2 ppm δ) = 2.15 Å
τ_c^0 = 0.0128 psec — r_{FF} (at -36 ppm δ) = 2.23 Å
r_{FF} (at -45 ppm δ) = 2.41 Å.

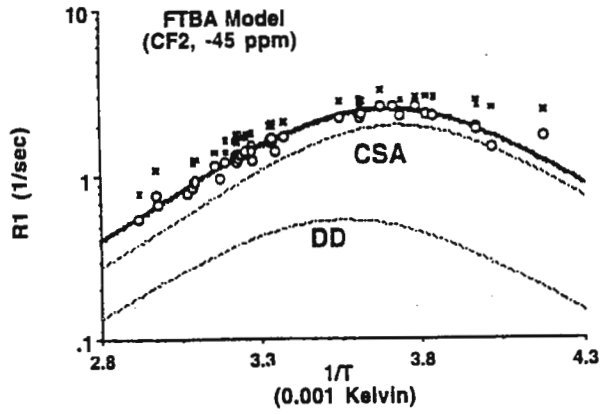
Then, we model the CF_3 data by using the above E_a and τ_c^0 values with r_{FF} = 2.25 Å and adjusting the E_{ai} and τ_{ci}^0 values of the internal motion to visually fit the data. Because the CF_3 T_1 minimum was not attained, our ability to characterize the CF_3 reorientation is limited. Ranges of E_{ai} and τ_{ci}^0 describe the data equally well: $3.3 \le E_{ai}$ (kcal/mole) ≤ 3.7 and $0.16 \le \tau_{ci}^0$ (psec) ≤ 0.23. These values are comparable to values in the ancient literature for CH_3 groups.

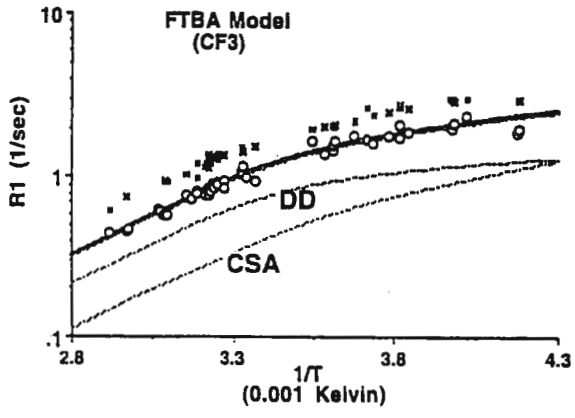
In this data modeling, we find that, at 7.05 tesla, the CSA contribution to the CF_2 $1/T_1$ is greater than the DD contribution, whereas, the reverse is true for the CF_3 $1/T_1$. Using the parameters given above, without any adjustment, we can reproduce the 9.4 tesla relaxation data that we made to validate our approach.

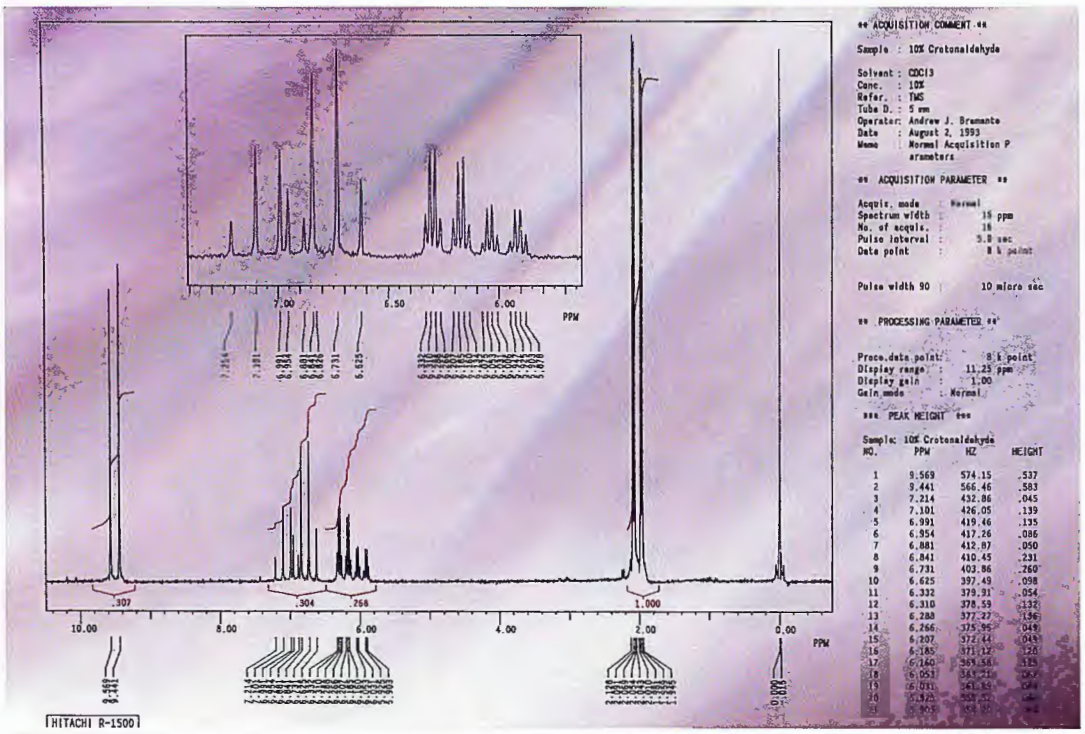
From the parameters given above, we find that τ_c at 25 °C is 193 psec. This "experimental" value is between the Stokes-Einstein-Debye value of 525 psec and the microviscosity-adjusted value of 88 psec. The agreement is encouraging. We tentatively interpret the low 88 psec value as due to an interlocking "cogwheel" effect that tends to correlate the reorientation of neighboring molecules.

The values of r_{FF} obtained in this analysis increase with increasing distance from the central nitrogen atom. We used COSY to identify the CF_2 resonances and found that the CF_2 group at -2 ppm is next to the N atom and that at -45 ppm is the farthest from N. This apparent increase in F-F distance might be caused by high frequency vibrations that average out part of the DD and CSA interactions; such motion should be greater for the outer CF_2 groups. For the inner CF_2 group, the agreement with the experimental, non-NMR, distance of 2.19 Å is excellent.

Donald E. Woessner — Himu P. Shukla — Ralph P. Mason







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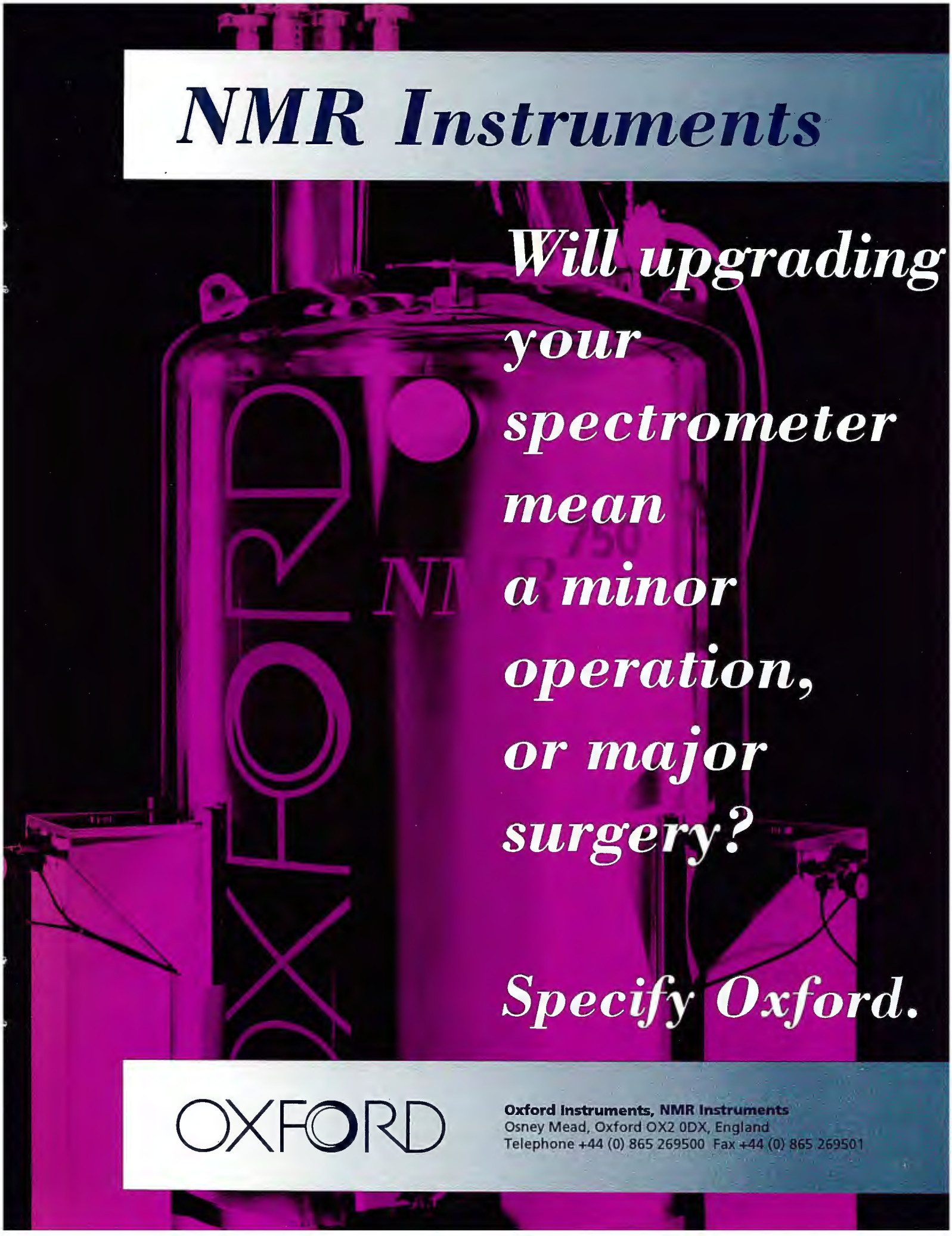
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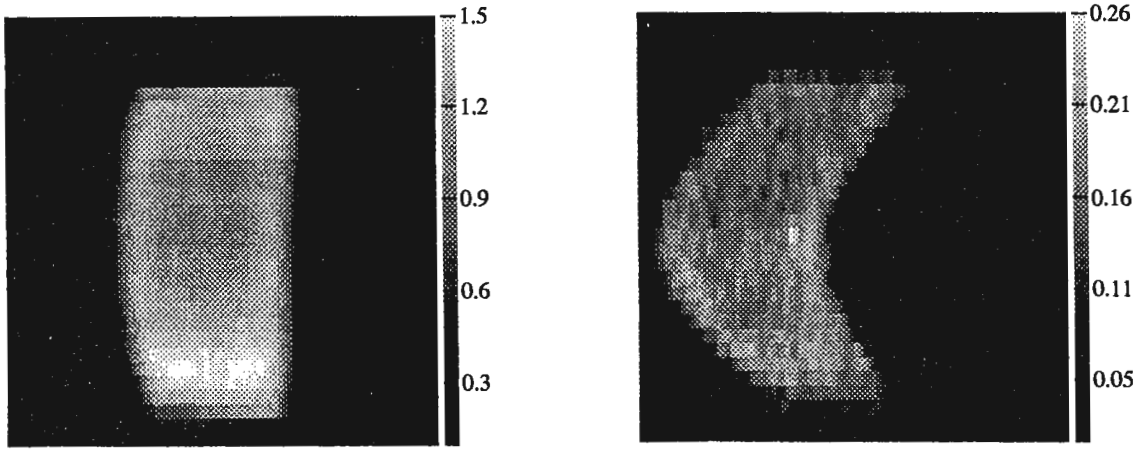
Dr. B.L. Shapiro
966 Elsinore Court
Palo Alto, CA 94303 U.S.A.

March 29, 1994
(received 4/23/94)

Imaging of flow and diffusion in flowing water.

Dear Dr. Shapiro,

In the framework of a study of diffusion techniques for in vivo NMR, we have applied Peter van Gelderen's single shot diffusion experiment [1] to flowing water. In an Oxford Instruments 4.7T superconducting magnet, equipped with Doty shielded gradient coils we had a 17 mm diameter tube with water flowing at about 6 mm/sec. Parallel to the direction of the flow a slice was selected with a 90- and a 180 degree RF pulse. With an alternating readout gradient (81 mT/m) following the 180 puls 15 gradient echoes were obtained. By repeating the experiment with 64 different values of a phase encoding gradient, which was applied in between the two RF pulses, we obtained 15 images of the flowing water with a time separation of 12.1 msec. Since the phase of the even echoes is compensated for flow, it should be possible to obtain the diffusion coefficient from their amplitudes.
In the Figure below you find images of the first and of the last echo. The displacement of the liquid due to the flow (from right to left in the images) is clearly visible. The difference in amplitude in the two images is mainly due to diffusion. Images of the phase also gave us the information on the flow and demonstrated clearly the flow compensation in the even echoes.



We obtained a diffusion coefficient of $(2.0 \pm 0.2)^* 10^{-5}$ cm^2/s, which is of the right order of magnitude, but we don't think that the results sofar are appropriate for in vivo application.

Please credit this contribution to Dr. Bovée's account.

Sincerely,

Patrick Bintevinos, Joris Creyghton

1. P.van Gelderen, A.Olsen, C.T.W. Moonen JMR A103, 105-108 (1993)

Departments of Radiology & Pathology
NMR LABORATORY

4301 West Markham, Slot 582
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501/686-6105
Fax 501/686-5406

Richard A. Komoroski, Ph.D.
Professor

UAMS MEDICAL CENTER

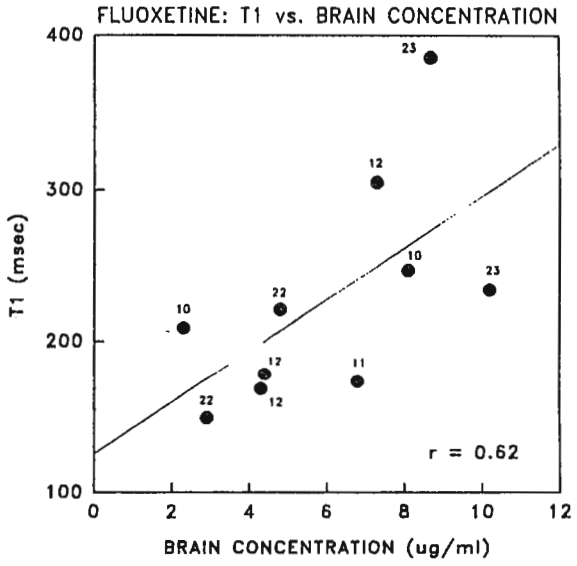
April 8, 1994
(received 4/12/94)
Dr. Bernard L. Shapiro
966 Elsinore Court
Palo Alto, CA 94303

Dear Barry:

For the last several years, my collaborators (Dr. C.N. Karson, Dr. J.E.O. Newton, D. Cardwell, J. Sprigg, and J. Pearce) and I have been using *in vivo* ^{19}F NMR spectroscopy to study psychoactive drugs in human brain. Several drugs used in the treatment of psychiatric conditions have fluorine as a part of their structure. The one most studied is the antidepressant fluoxetine (Prozac), which is widely prescribed and has received considerable press recently. We have measured drug concentration in the brain for 22 patients and achieved a crude localization of signal to brain (*Magn. Reson. Med.* 1994; 31:204-211, and references therein). To achieve a more reliable quantitation, we measured the ^{19}F T_1s *in vivo* in human brain in 5 patients (10 runs). The results are shown in the figure vs. the *in vivo* fluoxetine concentration. The numbers designate the patient in the overall study.

We were initially surprised to find a large variation in the ^{19}F T_1, even for the same patient at a different time. The quality of the T_1 fits, extensive T_1 measurements on phantoms, and a "true" *in vivo* repeat measurement (two runs on patient 12 at about 4 μg/ml separated by 1 day) lead us to believe that the T_1 differences are real, and not primarily experimental error. Measurements on the same patient at widely different times are not a reliable indicator of technique reproducibility because of changes in brain concentration, metabolism, and perhaps timing of the scan relative to adminstration of the drug. We found that the ^{19}F T_1 correlated weakly with brain concentration ($r = 0.62$, $p = 0.055$).

The behavior of T_1 with concentration can be rationalized on the basis of a simple exchange model for bound and unbound fluoxetine within the brain. At higher brain concentrations, more drug is not bound, is relatively free motionally, and has a higher T_1. The T_1 differences may also arise from varying relative amounts of fluoxetine and its major metabolite norfluoxetine, both of which contribute to the *in vivo* peak.



With best regards,

Richard A. Komoroski
Professor of Radiology and Pathology

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30 March 1994
(received 4/8/94)
Dr B. L. Shapiro
Tamu NMR Newsletter
966 Elsinore Court
Palo Alto, California 94303

Dear Dr Shapiro,

Neural Networks Used to Interpret PFG Diffraction-like Effects in Packed Arrays of Spheres

A diffraction-like effect has been observed in the PFG spin-echo (SE) NMR experiment when the echo attenuation, R, of a resonance arising from a species confined to the void volume of porous media is observed [1]. When R is plotted as a function of the wave vector q ($2\pi q = \gamma\delta g$; where g is the magnetic field gradient vector and δ is the duration of the field gradient pulse), the effect is manifest by a 'coherence' when the magnitude of q is equal to the distance between neighboring 'pores', b. We have observed this phenomenon in a packed bed of ~100 μm glass beads (Fig. 1) using a PFG longitudinal eddy current delay (LED) pulse sequence [2] to monitor H_2O diffusion in the pores of the bed. The mean glass-bead diameter, which was measured using image analysis of a scanning electron micrograph of the beads, was 105 ± 23 μm. For randomly packed spheres the value of b is approximately equal to the sphere diameter (e.g., [1]). The effective diffusion coefficient, D_{eff}, of the H_2O was estimated to be 1.40×10^{-9} m^2 s^{-1} from the low-q values of R. Non-linear least-squares (NLLS) regression of the pore-hopping equation for a pore glass [3] onto the values of R resulted in a low estimate of b (83 μm) but a reasonable estimate of D_{eff} (1.35×10^{-9} m^2 s^{-1}). Better estimates of b but poorer estimates of D_{eff} were obtained by performing NLLS regression analysis using values of logR; the estimated values of b (μm) were 95, 98, 103 and 106 for each of the diffusion times (s) of 2.5, 3.0, 3.5 and 4 and the mean value of D_{eff} was 0.7×10^{-9} m^2 s^{-1}. The differential performance of the two methods of analysis suggests that the model, for which the expression relating R to physical parameters of b, D_{eff} (and also pore radius) has been derived, may not adequately describe the physical system. It is possible that the 'pore equilibration' assumption that is fundamental to the pore-hopping analysis used here may not hold for packed spheres because the pores so formed can have complex shapes, have extremities separated by a distance as large as b and be connected to other pores via variable cross-section 'throats' rather than channels [4]. Therefore it is difficult to visualize that in the time taken for a molecule to diffuse a distance b, to a neighbouring pore, all the molecules remaining in the original pore may be found with equal probability anywhere in the pore irrespective of their starting position.

Monte Carlo simulations of diffusion can be performed without incorporating such assumptions [5, 6]. We have performed MC studies in which the diffusion of H_2O was simulated in the interstices of cubic-packed spheres. Simulations were performed for five different porosity values and six different b values (using diffusion times ~ $b^2 / 2 D_{eff}$; Fig. 2). The values of R, recorded as a function of q, from these simulations were used to train a three-layer feedforward neural network to predict the porosity and value of b in five MC-simulated test data sets. The mean error in the estimates for porosity and the value of b in the test data sets was 1.24% after 10,000 training iterations. In all test sets NLLS regression of the regular lattice pore hopping model [3] onto the values of R resulted in a value of b that was less than the value used for the simulation. The mean error of these estimates of b was 11%. We are currently using MC simulations to investigate diffusion in randomly packed spheres.

[1] Callaghan, P. T., Coy, A., MacGowan, D., Packer, K. J. and Zelaya, F. O. (1991) *Nature*, **351**, 467-469.
[2] Gibbs, S. J. and Johnson, C. S. (1991) *J. Magn. Reson.*, **93**, 395-402.
[3] Callaghan, P. T., Coy, A., Halpin, T. P. J., MacGowan, D., Packer, K. J. and Zelaya, F. O. (1992) *J. Chem. Phys.*, **97**, 651-662.
[4] Graton, L. C. and Fraser, H. J. (1935) *J. Geol.*, **43**, 785-909.
[5] Lennon, A. J. and Kuchel, P. W. (1994) *J. Magn. Reson. Series A*, in press for March.
[6] Piton, M. C., Lennon, A. J., Chapman, B. E. and Kuchel, P. W. (1994) *J. Colloid Interface Sci.* in press.

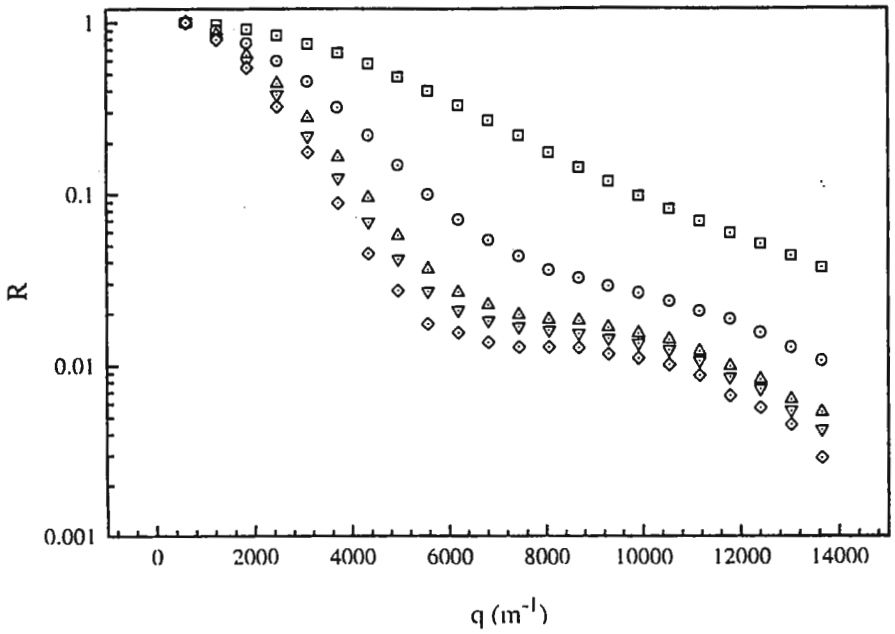

Figure 1. Echo attenuation of interstitial H_2O in packed glass beads recorded as a function of q. The data shown for diffusion times (s) of 0.5, □; 1.5, O; 2.5, Δ; 3.0, ∇; and 3.5, ◊, were the result of PFGLED experiments with τ = 30 ms, δ = 2 ms and g increments of 7.28 mT m^{-1}.

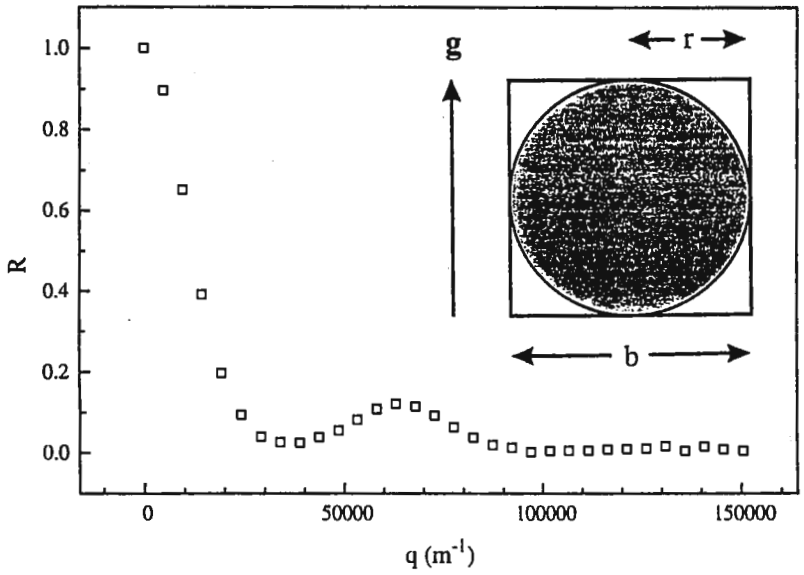

Figure 2. Model used for the MC simulation of diffusion of H_2O in cubic-packed spheres and typical simulated (n = 32) values of R obtained (b = 15 μm; porosity = 0.57). Different porosities were simulated by reducing the sphere radius and leaving the unit cell dimensions unchanged. Different values of b were simulated by altering the unit cell dimension.

Sincerely,

A. J. Lennon Philip W. Kuchel

Alison J. Lennon Philip W. Kuchel

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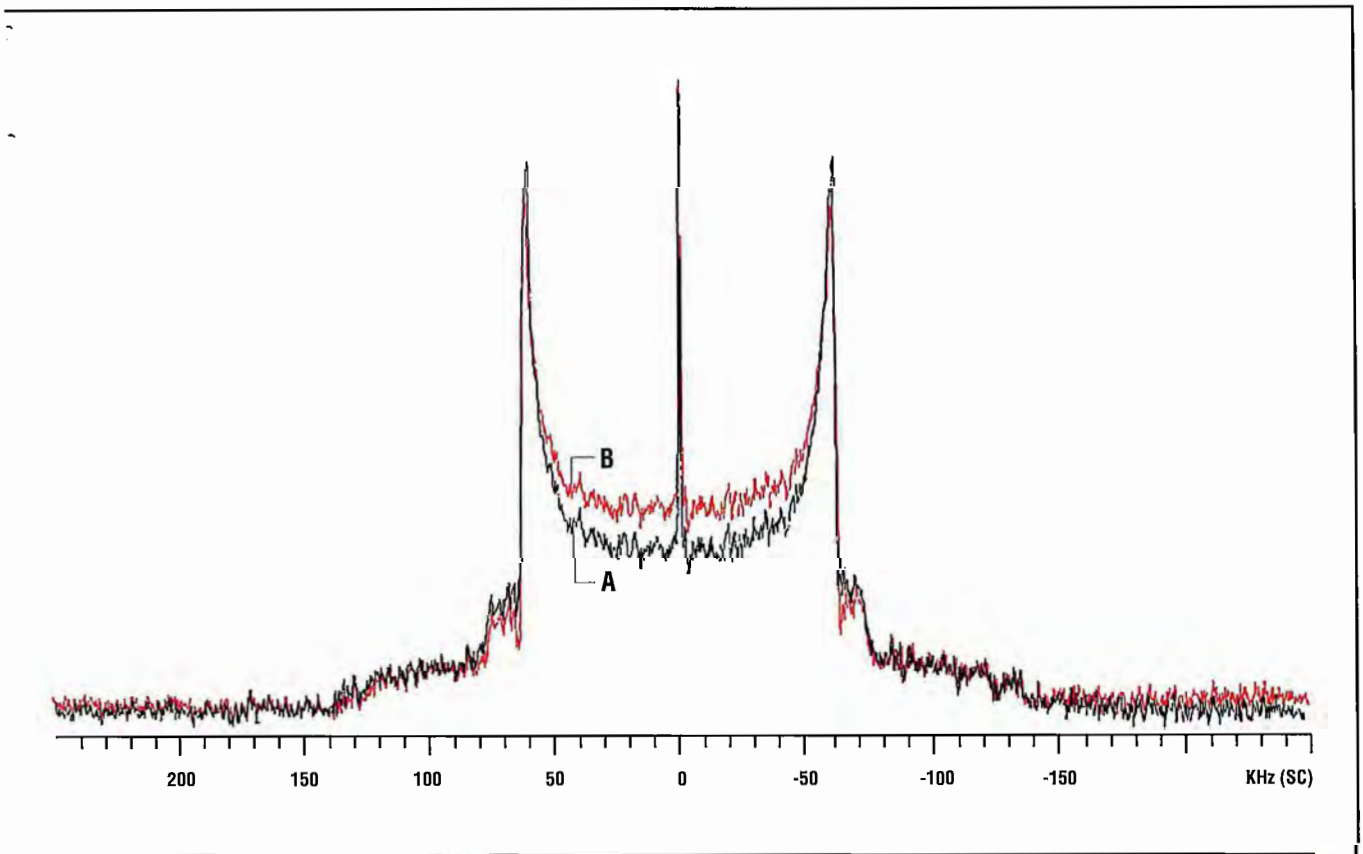

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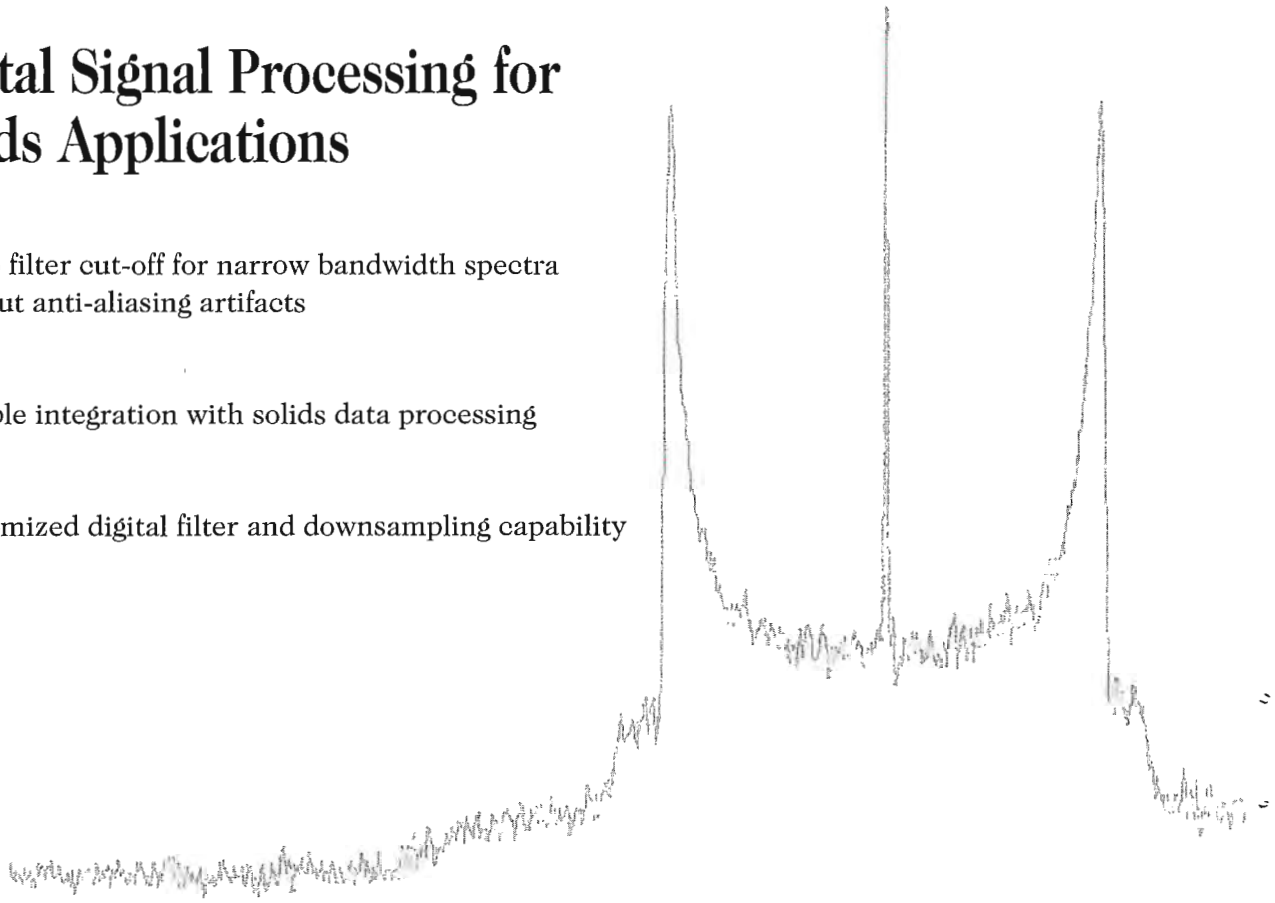

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Abbott Laboratories
One Abbott Park Road
Abbott Park, Illinois 60064-3500

March 31,1994 (received 4/9/94)

RE: Proline-edited HACA(CO)(N) experiment

Dear Dr. Shapiro:

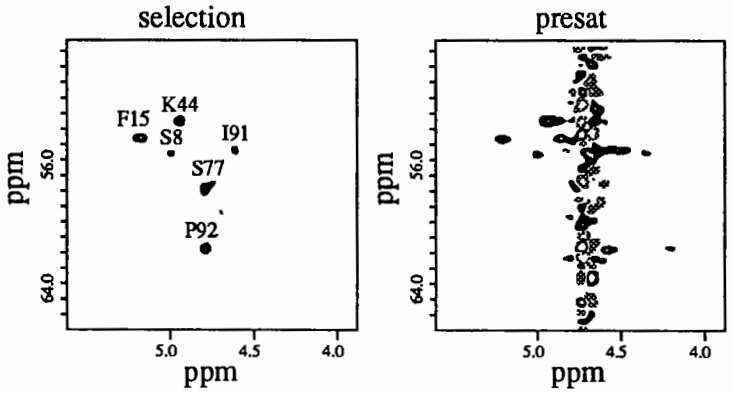
We recently developed a technique based on the 2D HACA(CO)(N) experiment which can be used to identify the H^{α} and C^{α} signals of the residues preceding prolines[1]. This experiment eliminates the signals corresponding to the non-proline residues by dephasing their ^{15}N magnetization by the one bond ^{15}N-^{1}H scalar coupling.

The major experimental obstacle in this experiment is to detect the desired H^{α} resonances in the presence of intense artifacts from the water signal. We initially attempted to do this experiment by using presat and gradients to suppress the artifacts from water, but as shown below (right), this was not a resounding success. However, much better suppression was obtained by using gradients for coherence selection of the desired resonances. This approach allowed us to identify six of the seven expected H^{α}/C^{α} resonances for the residues preceding prolines in FKBP.

Sincerely,

Ed Olejniczak, Steve Fesik

1. Olejniczak, E. T. & Fesik, S. W. J. Am. Chem. Soc. (1994) **116**, 2215-2216.



UNIVERSITY OF MISSOURI-ROLLA
Missouri's Technological University

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Department of Chemistry
142 Schrenk Hall
Rolla, Missouri 65401-0249
(314)-341-4451 (or 4420)
Bitnet - FBLUM @ UMRVMB
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Professor B.L. Shapiro
TAMU Newsletter
966 Elsinore Court
Palo Alto, CA 94303

March 26, 1994

Dear Barry:

NMR of POLYMERS
FACSS XXI and MMRS-5

The 21st Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Meeting will be held from Oct. 2-7, 1994 in St. Louis, MO, USA. Held jointly with this meeting will be the 5th Missouri Magnetic Resonance Symposium (MMRS) on Wednesday (Poster session, PM) and Thursday (oral sessions, AM, PM) of that week.

Contributed papers are now being solicited for this symposium in all areas of magnetic resonance. Student posters are especially of interest. Students giving posters in the MMRS poster session (Wed. PM) are eligible to apply for a stipend ($35) to cover registration costs for the entire FACSS meeting. A copy of the abstract of the poster presentation should be sent to F.D. Blum to apply for these. There are a limited number, so interested students need to apply soon.

Currently, the list of invited speakers includes: H.N. Cheng (Hercules), P. Smith (Dow), J. Garbow (Monsanto), F. Blum (Missouri-Rolla), C. Wade (IBM), S. Kaplan (Xerox), J. Miller (NRL), N. Zumbulyladis (Kodak), J. Schaefer (Washington U.), and T. Cosgrove (Bristol).

For registration and abstract materials, contact: FACSS National Office, 198 Thomas Johnson Dr., Suite S-2, Frederick, MD, 21702-4317, USA. (310-846-4797).

Sincerely,

Frank

Frank D. Blum
Curators' Professor of Chemistry
and Senior Investigator
Materials Research Center

NMR Spectroscopist Looking for a Job

Jacques Reuben, a seasoned and well-published NMR spectroscopist/analytical scientist, has lost his employment in the recent corporate downsizing and **is looking for a new job.** He has 14 years of industrial experience in analytical problem solving, molecular structure determination, chemical kinetics, and reaction mechanisms. Broad background includes physical chemistry, biophysical chemistry, organic chemistry, inorganic chemistry, and biochemistry. Experience with phosphazenes, cyclodextrins, ESR spectroscopy, free radicals in polymers, disposability of plastics. Particular expertise in:

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- Cellulose ethers - Process evaluation through product analysis
- Structure of water soluble polymers
- Analysis of paper chemicals: wet strength resins and sizing agents
- Kinetics of substitution reactions
- Interaction between small molecules/ions and biopolymers
- Lanthanide shift and relaxation reagents

A recent analysis of his accomplishments indicates that Jacques has strong analytical skills with the ability to be persistent and disciplined in his pursuit of an objective where he can apply persuasion and is willing to take reasonable risk.

Jacques is willing to relocate. If you can help him in his job search please call him at (302) 478-5860 or write to him at 38 Club Lane, Wilmington, DE 19810-3309.

GRADIENT SHIMMING

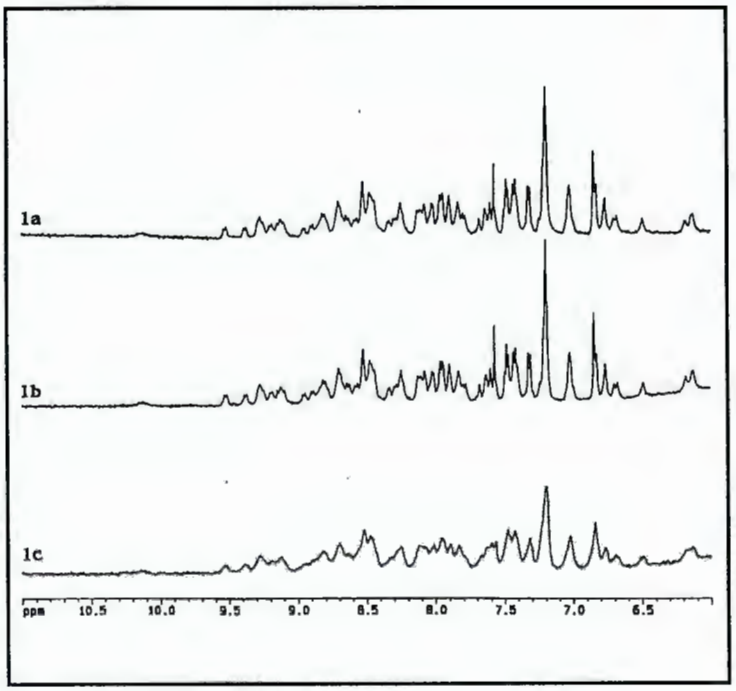
BRUKER

Optimization of magnetic fields is crucial for high resolution NMR spectroscopy. So far the approach to shimming the field is pragmatic, slow and dependent on the operators skill and endurance. Now Bruker has adapted an auto shimming technique, which is currently used on diagnostic MRI systems, to facilitate the shimming of high resolution samples.

Automatic homogeneity adjustment of the x,y,z shims can be done using a three dimensional phase mapping technique as used by whole body imaging systems. For each automatic iteration, we acquired a 3D data set (64 x 32 x 32 increments) which takes ca. 10 minutes. The known shape and corrections of the actual shim system are then used together with these results to calculate an optimal shim setting for the sample. Following this, a 1D NMR experiment can be done to check the resulting magnet homogeneity.

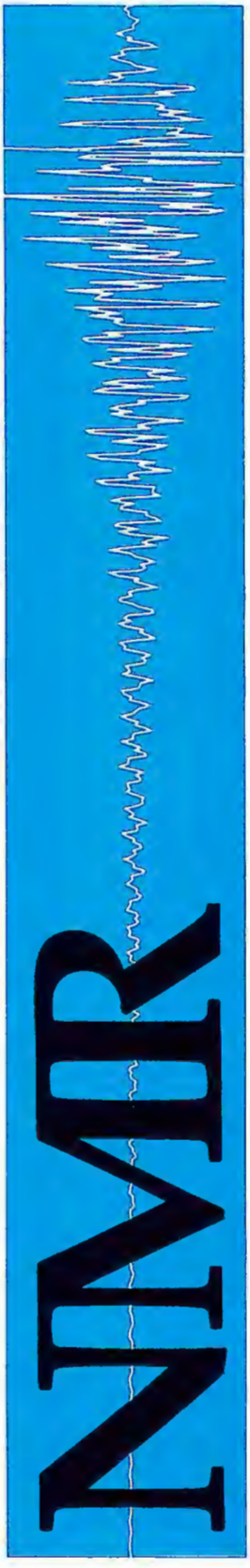
We have applied this technique at 500 MHz using the Bruker 5 mm TXI (inverse triple resonance) GRASP-III (GRAdient SPectroscopy with x,y,z-gradients) probe, together with the BOSS-II shim set (using Z1-Z6 and 12 off-axis gradients) and found that it can dramatically improve the field homogeneity and reduce the time needed to reach optimal field homogeneity.

Our results show that gradient shimming can be extremely successful, quick, and give results that are as good or better than those produced by experienced spectroscopists. As an example, the 1D proton spectrum of 2 mM ubiquitin (90% H_2O/10% D_2O), following conventional shimming is shown in Figure 1a.



We then deliberately misset the major shim values to give the poorly shimmed spectrum shown in figure 1c.

After one iteration of the automatic gradient shimming procedure, we obtained on first try, a spectrum shown in Figure 1b, that is as good as the spectrum shimmed by the spectroscopist.



We then applied the automatic gradient shimming technique to the sucrose water suppression sample (2 mM sucrose in 90%H_2O/10%D_2O, with DSS for reference). The standard Bruker parameters for presaturation of the water resonance and acquisition of the data were used following the gradient shimming. We reached a more than satisfactory result following the third iteration of the automatic gradient shimming, such that the line width of the residual water resonance after presaturation (at 50% height of the DSS signal) is <53 Hz.

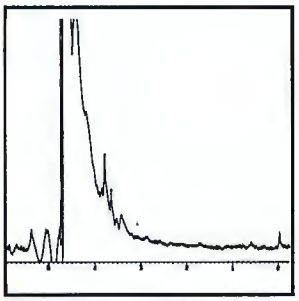


Figure 2a: TIME = 0, shims not optimized.

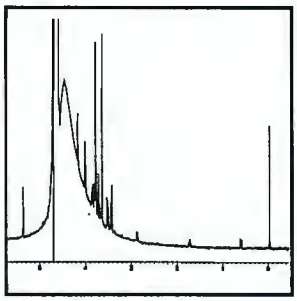


Figure 2b: FIRST iteration.

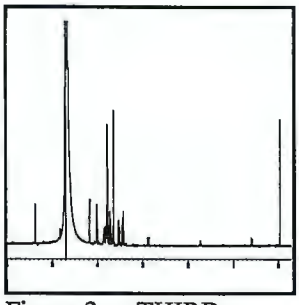


Figure 2c: THIRD iteration.

An additional example is shown for our results using a sample of BPTI (1.5 mM in 90%H_2O/10%D_2O). A 1D proton experiment (16 scans, 2 dummy scans) was acquired with a 1.3 second water presaturation. After a second iteration of the gradient shimming routine, we achieved very respectable results.

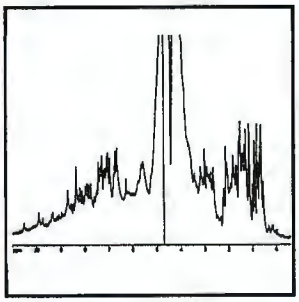


Figure 3a: TIME = 0, using starting shim values.

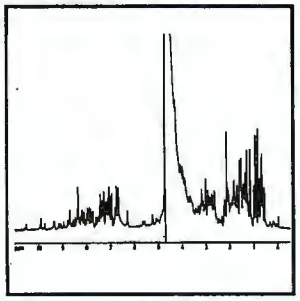


Figure 3b: FIRST iteration, with a clear improvement in the water linewidth.

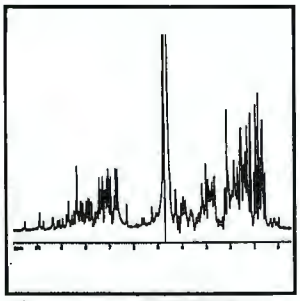


Figure 3c: SECOND and final iteration gives good resolution and linewidth.

These examples show that it is possible to perform successful gradient shimming on 5 mm samples with the Bruker GRASP-III probes within a short period of time and with excellent results. This technique offers promise for the challenges of shimming more difficult sample volumes, such as 2.5, 8.0 and 10 mm samples, or even 5 mm samples with a short filling height.

BII 3/94, P.van Zijl, M. O'Neil-Johnson, S. Sukamar, R. Hurd, P.Webb

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April 26 1994

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

Dynamic NMR, as Manifest in Relaxography

Dear Barry:

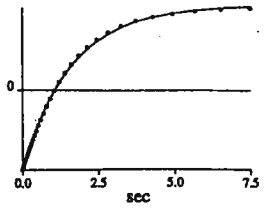
Chemists have long been intrigued by the effects on the spectrum of the facile equilibrium exchange of spins between two or more environments with different resonant frequencies. This phenomenon has been termed *Dynamic NMR* (DNMR) *spectroscopy*. Of course, there are many situations in which there is no dispersion in frequency. Since 1991, we have been advocating that the distribution of relaxation times - what we like to call the *relaxogram* - has some of the attributes of the spectrum.[1] In many ways, it is another dimension for NMR - and there is one for each kind of relaxation time: T_1, T_2, and $T_{1\rho}$. The relaxogram is formally the inverse Laplace Transform (ILT) of the relaxation decay data set - and its study can be termed *relaxography*.

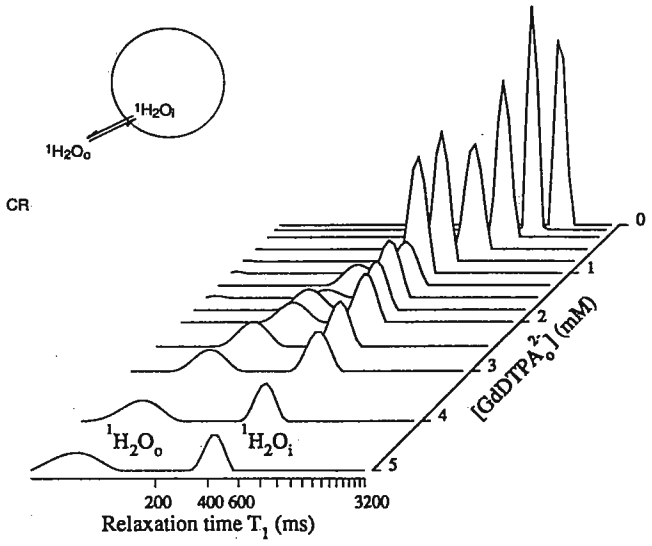
The Figure illustrates the manifestation of DNMR in relaxography.[2] Panel A shows a stacked plot of longitudinal relaxograms obtained (at 9.4 T) for the ^1H_2O signals of suspensions of yeast cells with densities averaging 3.43 ($\pm$ 0.16) x 10^9 cells/mL but containing different concentrations of the clinical MRI contrast reagent (CR), $GdDTPA^{2-}$, in the extracellular space. For the relaxogram of the suspension with no CR, the ^1H_2O inversion recovery data are shown above the stacked plot. The top relaxogram is the formal ILT of these data, and the solid line through them is the LT of the top relaxogram. The data for the suspension with 5 mM CR are shown at the bottom of the stacked plot and they bear an analogous relationship with the bottom relaxogram.

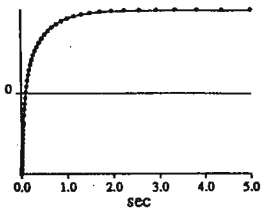
The facts that the single relaxographic peak observed in the absence of CR shifts to smaller T_1 values with increasing $[CR_o]$ before being resolved into two peaks, and that, after this, the relative area of the peak with smaller T_1 (assigned to $^1H_2O_o$) increases at the expense of that of the peak with longer T_1 (assigned to $^1H_2O_i$) are clear indications of the presence of equilibrium transcytolemmal exchange of the water proton spins. Although $GdDTPA^{2-}$ does not cause a shift in the resonance frequency of ^1H_2O, it does shift the T_1 of the extracellular spins to a smaller value. The theory for exchange between two environments with different relaxation times but the same resonant frequency has been known since McConnell modified the Bloch equations in 1958.[3] Panel B shows a fitting of the relaxographic results of panel A with a two-site exchange model having five independent variables: the T_1 value of $^1H_2O_o$ in the absence of CR, T_{1o0}, the T_1 value of $^1H_2O_i$, T_{1i}, the relaxivity of extracellular CR, r_{1o}, the fraction of ^1H_2O that is intracellular, p_i (= 1-p_o), and the average pre-exchange lifetime of intracellular ^1H_2O spins, τ_i (= $\tau_o(p_i/p_o)$). The observable quantities are: the position of the relaxographic peak at the smaller T_1 value, T_{1S}, the position of the peak at the larger T_1 value, T_{1L}, and the relative area of the peak at the smaller T_1 value, a_S (= 1-a_L). The widths (and heights) of the relaxographic peaks are not particularly meaningful, because of the regularized nature of the numerical ILT procedure used.[2] In panel B, a plot of T_1^{-1} versus $[CR_o]$, the T_{1S}^{-1} values are given as open circles, the T_{1L}^{-1} values as filled circles, and the a_S/a_L ratio values are given (in the inset) as open diamonds. The three solid curves are the theoretical values for these quantities from a four-parameter fitting. With T_{1o0} held constant at 2.22 s, the values for the other four variables corresponding to the fitting are: T_{1i} = 0.942 s, r_{1o} = 2.35 $s^{-1}(mM)^{-1}$, p_i = 0.36, and τ_i = 0.672 s. The last two are in good agreement with literature results.[2]

There are two major differences between *DNMR relaxography* and DNMR spectroscopy. The first is the *change* in relative areas of the two relaxographic peaks (inset of panel B). This does not happen in DNMR spectroscopy during coalescence, or emergence therefrom. The second is the fact that because of rapid exchange, the two observed T_1 values are each smaller than their respective true T_1 values (the dashed curves for r_{1o} and T_{1i}^{-1} are each lower than their respective solid curves in panel B). In DNMR spectroscopy, the observed

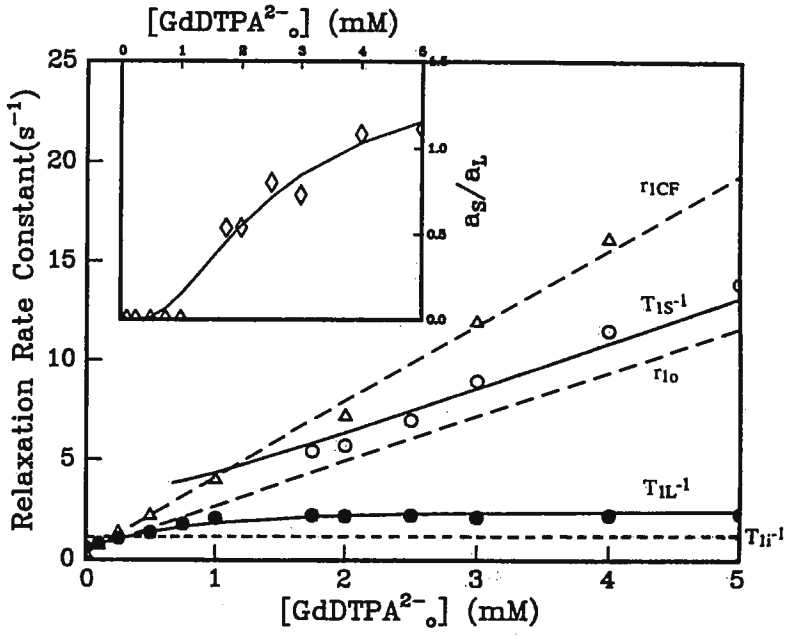
A







B



1. C. Labadie, T. M. Button, W. D. Rooney, J-H. Lee, and C. S. Springer, *Abstr. 10th Ann. Mtg. Soc. Magn. Reson. Med.*, Soc. Magn. Reson. Med., Berkeley, CA; p. 1218 (1991).
2. C. Labadie, J-H Lee, G. Vetek, and C. S. Springer, *J. Magn. Reson.*, in press (1994).
3. a. H. M. McConnell, *J. Chem. Phys.* 28, 430 (1958). b. D. E. Woessner, *J.C.P.* 35, 41 (1961). c. J. S. Leigh, *J. Magn. Reson.* 4, 308 (1971). d. A. C. McLaughlin, and J. S. Leigh, *J.M.R.* 9, 296 (1973).
4. S. R. Tanny, M. Pickering, and C. S. Springer, *J. Am. Chem. Soc.* 95, 6227 (1973).
5. I. Palyka, M. S. Albert, and C. S. Springer, *Abstr. 12th Ann. Mtg. Soc. Magn. Reson. Med.*; Soc. Magn. Reson. Med.; Berkeley, CA; p. 778 (1993).

resonance frequencies are always intermediate between those operative in the absence of exchange. Compare this Figure with the results of a DNMR spectroscopic experiment we reported in the Dark Ages,[4] which is quite analagous to that here.

In the *in vivo* context, we have seen ^1H_2O T_1 relaxograms such as those shown in panel A after the injection of $GdDTPA^{2-}$ into mice.[5] When we include spatial encoding in the pulse sequence - *combined relaxography and imaging* - we can obtain very interesting results. An image made from only the spins represented by one relaxographic peak can be called a *relaxographic image*.[2] The relaxographic image from the $^1H_2O_o$ peak is a direct image of the distribution volume of the CR. It is an extracellular map of most tissues and a plasma (or vascular) map of the healthy brain, since the blood-brain-barrier constrains the CR to the plasma. The relaxographic image from the $^1H_2O_i$ peak is a parenchymal map of the healthy brain and a cytoplasmic volume map of most tissues. The latter will allow the determination of the *thermodynamic* concentrations of intracellular metabolites *in vivo*, and in a relatively noninvasive manner. Conversely, we can observe relaxograms from single imaging voxels of less than 500 nL nominal volume. This is because the ^1H_2O signal is by far the strongest from tissue. These localized relaxograms can allow a good estimate of the thermodynamic value of $[CR_o]$ in the voxel. In this context, the T_{1S}^{-1} curve in panel B can be used as a calibration curve and it is important to note that it is not the same as that obtained for a simple aqueous (cell-free) solution ($r_{1CF} = 3.81\ s^{-1}(mM)^{-1}$, open triangles and dashed line in panel B).

Best regards,

Charlie

Jinghui Lee

Charles S. Springer, Jr.
Chemist/Professor of
Chemistry, USB

Jing-Huei Lee
Postdoctoral Associate
Center for Magnetic
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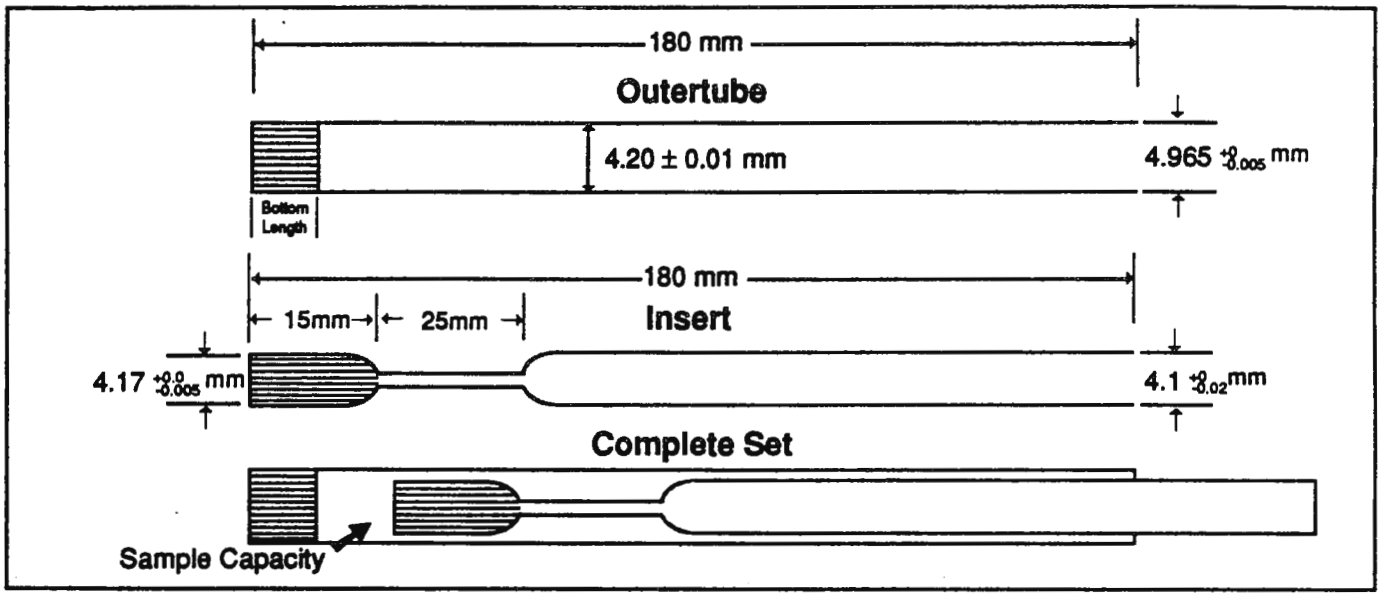

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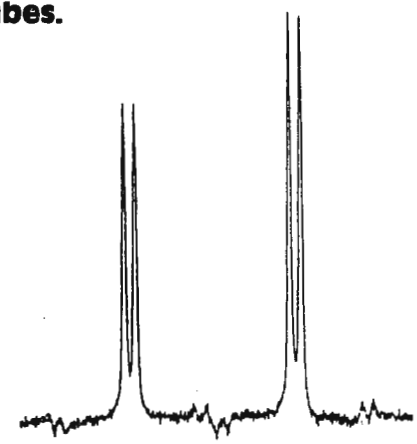

Fig.1a Fig.1b

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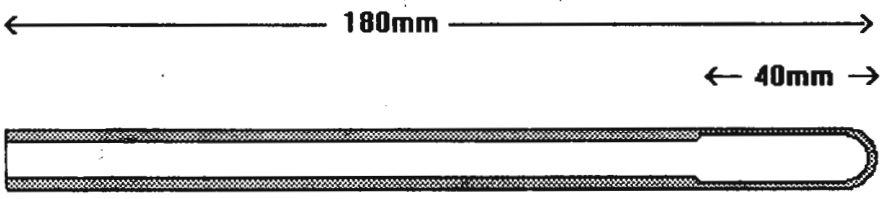

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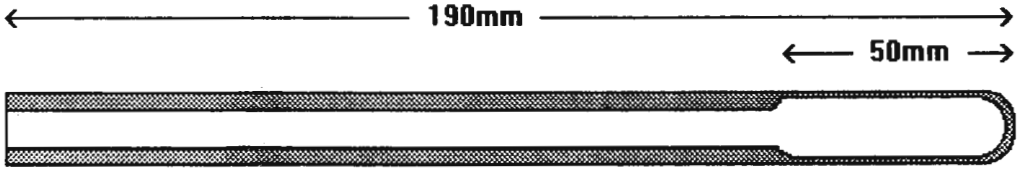

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FORTHCOMING NMR MEETINGS, *Continued from page 1.*

Symposium on "NMR as a Structural Tool for Macromolecules: Current Status and Future Directions, Indianapolis, IN, **October 30 - November 1, 1994**; Contact: Ms. Padmini Nallana, Coordinator, NMR Symposium, Dept. of Physics, Indiana University Purdue University Indianapolis, 402 N. Blackford St., Indianapolis, IN 46202-3273; Tel. (317) 278-1263; E-mail: PADMINI@INDYVAX.IUPUI.EDU; Fax: (3172) 274-2393. See TAMU NMR Newsletter 425, 31.

36th ENC (Experimental NMR Conference), Boston, MA, **March 26 - 30, 1995**; Contact: ENC, 815 Don Gaspar, Santa Fe, NM 87501; (505) 989-4573; Fax: (505) 989-1073

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**; Contact: Dr. Les. Field, Dept. of Organic Chemistry, Univ. of Sydney, Sydney, NSW 2006, Australia. Phone: +61-2-692-2060; Fax: +61-2-692-3329; Email: ismar-95@biochem.su.oz.au Also, see TAMU NMR Newsletter 419, 26.

Additional listings of meetings, etc., are invited.

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

Deadline Dates

No. 430 (July)	24 June 1994
No. 431 (August)	22 July 1994
No. 432 (September)	26 August 1994
No. 433 (October)	23 Sept. 1994

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