THE
NMR
NEWSLETTER

No. 493

October 1999

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FORTHCOMING NMR MEETINGS

NMR Technologies: Development and Applications for Drug Discovery, Baltimore, MD, **November 4-5, 1999**; Contact: Cambridge Healthtech Institute, 1037 Chestnut St., Newton Upper Falls, MA 02464; el. 617-630-1300 or (in U.S.) 888-999-6288; Fax. 617-630-1325; e-mail: chi@healthtech.com; www.healthtech.com; See Newsletter 493, 24.

Medical Imaging: NMR and Nuclear Tracers, colloquium at the 12th Entretiens Jacques Cartier, Lyon, France, **December 5-8, 1999**; See http://jade.univ-lyon1.fr/JacquesCartier/ and Newsletter 488, 38.

Biennial Meeting of the Australian and New Zealand Society for Magnetic Resonance (ANZMAG2000), Mt. Buller, Victoria, Australia; **February 13-17, 2000**; Contact: Dr. Jenny Wilson, Victorian College of Pharmacy, Monash University, Parkville, Victoria 3052, Australia; E-mail: anzmag@edda.vcp.monash.edu; vcp.monash.edu.au/chemistry/anzmag2k.

PITTCON 2000, New Orleans, LA, **March 12-17, 2000**; Contact: The Pittsburgh Conference, 300 Penn Cemter Blvd., Suite 332, Pittsburgh, PA 15235-5503; Phone: 412-825-3220; Fax: 412-825-3224; Email: expo@pittcon.org.

8th Scientific Meeting and Exhibition, International Society for Magnetic Resonance in Medicine, Denver, CO, **April 1-7, 2000**; Contact: ISMRM, 2118 Milvia Street, Suite 201, Berkeley, CA 94704. Tel. 510-841-1899; Fax. 510-841-2340; E-mail: info@ismrm.org; http://www.ismrm.org.

41st ENC (Experimental NMR Conference), Asilomar Conference Center, Pacific Grove, CA, **April 9-14, 2000**; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87505; (505) 989-4573; Fax: (505) 989-1073; E-mail: enc@enc-conference.org. Web: enc-conference.org

15th European Experimental NMR Conference, Leipzig, Germany, **June, 2000**. For information, see http://eenc.uni-leipzig.de.

SMASH-2000, Argonne, IL, **July 16-19, 2000**. Contact: G. E. Martin (gary.e.martin@amu.pnu.com). See Newsletter 493, 21.

XIX International Conference on Mag. Res. in Biological Systems, Florence, Italy, **August 20-25, 2000**. Contact: Profs. Ivano Bentini or Lucia Banci, Chem. Dept., Univ. of Florence, Via G. Capponi 7, I-50121, Florence, Italy; Phone: +39-055-2757600; Email: icmrbs@lrm.fi.cnr.it; Fax: +39-055-2757555; http://www.lrm.fi.cnr.it//icmrbs.html.

Royal Society of Chemistry: 15th International Meeting on NMR Spectroscopy, Durham, England, **week of July 8-13, 2001**; Contact: Mrs. Paula Whelan, The Royal Society of Chemistry, Burlington House, London W1V 0BN, England; +44 0171 440 3316; Email: conferences@rsc.org\

Additional listings of meetings, etc., are invited.

KUNGL
TEKNISKA
HÖGSKOLAN

Department of Chemistry, Physical Chemistry
Professor Peter Stilbs

(received 9/22/99)
Stockholm September 20, 1999

Page 1 of 1

Professor B.L. Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto
CA 94303-3410
USA

Re: CORE for PC and Alpha (OpenVMS and NT) available for download

Dear Barry,

Thank you for your orange Ultimatum. Since March 1999 the CORE (1-3) program (OpenVMS Alpha, 'Intel PC' and 'Alpha (NT) PC' versions) has been freely available from my homepage indicated below. This is presently not a 'windows program', however (it runs in a 'DOS window'). Graphics display through Matlab is supported. Pentium II or III computers show quite reasonable processing times (about twice those of Alpha's with the same clock frequency).

CORE (Component Resolved Spectroscopy) is a useful computational procedure that utilizes all available information in data sets of 'kinetic type', i.e. where component bandshapes stay constant but undergo common and known/testable intensity changes. CORE was originally developed for analyzing multi-component FT-PGSE NMR self-diffusion data in the case of severe spectral overlap, but can often easily be adapted for other problems. The present version of CORE has working interfaces for importing Bruker AMX/DMX type data, and pure ASCII files (like from spreadsheets or Matlab). Through the kind help of Rolf Kyburz of Varian I also have access to Varian data sets, and hope to get time to work on some type of interface for reading those as well. Future CORE versions may include provisions for 'DOSY display' of FT-PGSE results.

Yours Sincerely

Peter

Peter Stilbs

1. P. Stilbs, K. Paulsen, P. C. Griffiths, "Global Least-Squares Analysis of Large, Correlated Spectral Data Sets: Application to Component-Resolved FT-PGSE NMR Spectroscopy", J. Phys. Chem. 100, 8180 -8189.(1996). 2. P. Stilbs, K. Paulsen, "Global least-squares analysis of large, correlated spectral data sets and application to chemical kinetics and time-resolved fluorescence", Rev. Sci. Instrum. 67, 4380 -4386.(1996). 3. P. Stilbs, "Component separation in nmr imaging and multidimensional spectroscopy through global least-squares analysis, based on prior knowledge", J. Magn. Reson. 135, 236 -241.(1998).

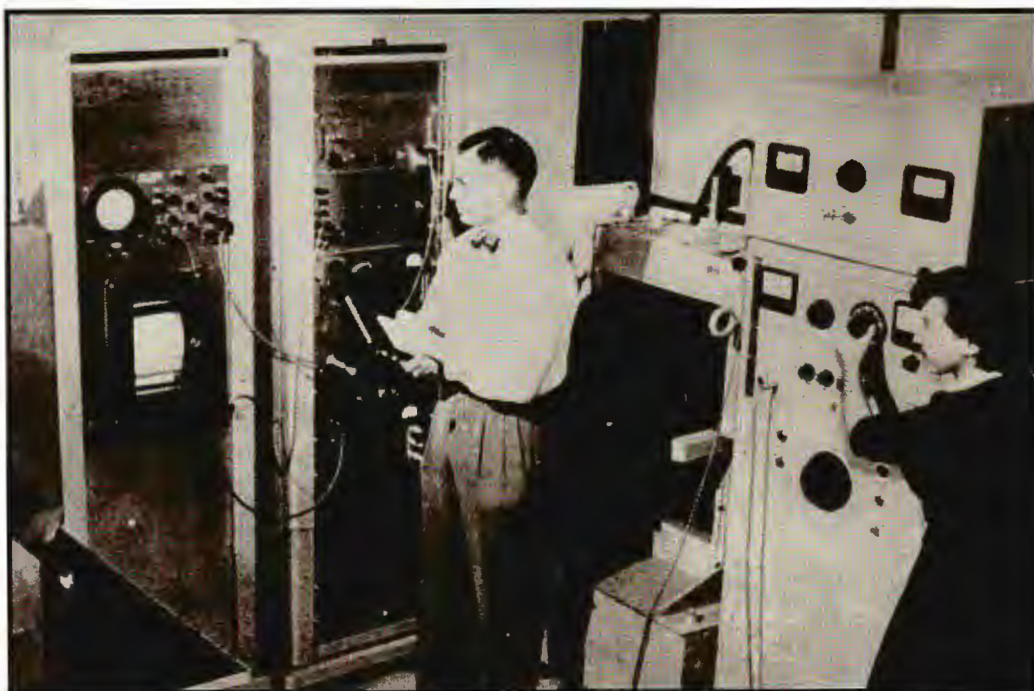| Postal address:	Visiting address:	Telephone:		E-mail:
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From left to right:

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Earthy Lee Young
Remonda Lavinghouse
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McMaster
University

September 9, 1999   (received 9/13/99)

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

WEAK COUPLING IN EXCHANGE, PRO AND CON

Dear Barry:

We are still trying to make chemical exchange lineshape calculations as simple and efficient as we can. Our MEXICO program is progressing (things always take longer than you think), and I hope that by the time this gets published, a new version will be available. However, as we have been developing it, the usual tradeoffs between speed and accuracy start to arise.

A couple of the improvements over Binsch's landmark DNMR3 program are a more exact description of the T_2 effects on lines, and the possibility of weak coupling. With T_2 properly treated, we can get an essentially exact simulation of the lineshape. However, as with most simulations, the time required for the calculation rises steeply just as the spin systems start to get interesting. Table 1 gives some data obtained on a rather old SGI Indy computer.

Table 1: Two-site Non-mutual Exchange, Strong Coupling			
Spin System	Total Matrix Size	Largest	Time (s)
ABCD	112	48	2.5
ABCDE	420	200	56
ABCDEF	1584	600	3230

For a strongly coupled ABCD system with two sites, there are 56 transitions in each site, giving a 112 x 112 complex matrix to be diagonalized. Factoring on the F_z quantum number breaks the system into blocks, the largest of which is 48 x 48. All of this ends up taking about 2.5 seconds. However, standard matrix diagonalization scales as the cube of the size of the matrix. Adding a spin increases the size of the matrix by roughly a factor of 4, so that costs us a factor of 64 in time, as we can see in the table. Doing the matrix manipulations in less standard ways can avoid some of this rather frightening scaling (next year's letter!), but the temptation is to use a weak coupling approximation to reduce the matrix size as well.

Table 2 shows what you can do with weak coupling. The reduction in size comes from the loss of combination transitions, which are almost always negligible. In the table, the spaces between the letters indicate weak coupling, so AB CDE is really an ABXYZ system in proper Pople notation.

| Table 2: Strong *vs* Weak Coupling			
Spin System	Total	Largest	Time (s)
ABCDE	420	200	56
A B C D E	160	60	9.1
A BCDE	364	168	42.5
AB CDE	340	156	31.1
AB CD E	264	116	18.1

In fact, the fully weakly coupled system can be treated as a bunch of 2 x 2 exchanges, so it can be done quite efficiently.

But remember that weak coupling gives reliable frequencies (usually), but not very good intensities. Line positions are perturbed only to second order, but intensities are perturbed to first order. In spite of the seductive nature of the numbers in Table 2, we usually try to keep all the strong coupling, at least towards the end of a fitting procedure. If you really need the speed, buy a faster computer, or do your matrix manipulations by some method other than Householder.

Yours truly,

Alex D. Bain
Professor of Chemistry
bain@mcmaster.ca
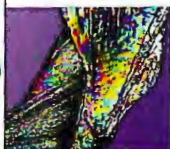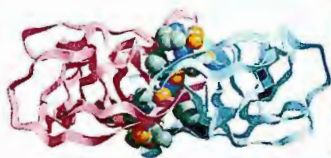
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Attempts to Apply Large Sideband Corrections to CPMAS Spectra

Tom Pratum, Department of Chemistry, University of Washington, pratum@u.washington.edu

Carbon-13 CPMAS NMR is an important tool for the analysis of carbon functional groups in natural organic matter. Tempering the optimism for the use of this technique are quantitation, and S/N problems. The tried and true method for obtaining these spectra is to operate at a low field and moderate spinning rate so as to reduce the possibility of spinning sidebands while not having to spin at a rate such that cross polarization is adversely affected. The recovery of S/N in these low field spectra has been dealt with by increasing the sample size through the use of large volume spinning assemblies *(1)*. For many NMR laboratories, it is not possible to justify acquisition of a separate low field NMR spectrometer with a specialized spinning assembly for solids work, so they have attempted to acquire these data on their existing high field spectrometers; in some cases at fields up to and including 14 Telsa (600 MHz ^{1}H) (*see e.g. ref 2*). Acquisition of these spectra at such high fields appears to be ill-advised, but occurs nonetheless. In situations where the researchers employing high field strengths are unable to spin adequately, TOSS is sometimes used to remove the sidebands from the spectra. TOSS is clearly not a quantitative technique, and this further muddies any conclusions to be drawn from such work.

Several years ago we showed that CPMAS spectra with moderate levels of sideband interference could be corrected by using measured chemical shift anisotropy (csa) parameters from similar materials to predict the sideband intensities, and use those sideband intensities to correct the measured integral areas *(3)*. To do this, we first performed the standard CPMAS experiment at a spinning rate such that the selected regions were separated by an integral number of spin rates. In what is shown here the regions were 15 ppm wide and covered the range 210-0 ppm, or 198–12 ppm (14 regions total numbered 0-13 with 0 being the most downfield). The sidebands were analyzed over these regions either by re-integrating the previously obtained sideband data (acquired using the method of Feaux deLacroix *et al.* *(4)* at a spinning rate of 3200 Hz), or re-measuring the sidebands for the sample of interest using the 5 pulse PASS method of Levitt *et al.* *(5)* at a slower spinning rate (2000 Hz). The analysis of the sideband intensities was accomplished using the very nice Mathematica notebook which is provided on the Levitt group website (http://www.fos.su.se/physical/mhl/science/research.html). These sideband intensities (up to third order) are then entered into the system of linear equations which describes how the centerbands and sidebands add to create the observed spectrum:

$$A \cdot B_o = B,$$

where A is a 14x14 matrix of normalized sideband intensities determined from the chemical shift parameters of each region and arranged with the rows indicating the sideband contribution to each region, and the columns containing the sideband intensities which originate in a particular region. The column vector B_o contains the (unknown) centerband intensities, and B is a column vector of the observed uncorrected integral intensities of the standard CPMAS experiment. The matrix equation $A \cdot B_o = B$ does not give the corrected intensities directly. After B_o is obtained, by numerical elimination, or a similar method, corrected integrals are generated by multiplying each element of B_o by the sum of normalized sideband intensities for that region. For example, the corrected intensity of region (a) would be:

$$(1 + a_{-3} + a_{-2} + a_{-1} + a_1 + a_2 + a_3)a_o,$$

where the subscripts indicate the sideband order. The question here is whether this procedure can be used for the larger sideband corrections which might be needed when operating at very high field.

1

As a test, CPMAS spectra were acquired at 3 spinning rates which were multiples of 15 ppm for ^{13}C at 7.0 Tesla (2264, 3396, and 4528 Hz), and these were corrected as outlined above. We show below the resulting areas obtained from a series of standard 1 msec contact CPMAS spectra obtained at 3 different spinning rates on a fulvic acid from a shrub/sedge wetland in Western Washington. As can be seen, when the correction is applied using the csa parameters which were used in the previous study, there are wild deviations from reasonable integral area values in the corrected data for the slowest spinning rate. Since these csa parameters were obtained from ssb intensities at a spinning rate of 3200 Hz, it was thought that perhaps extrapolation of the values to obtain sideband intensities at much lower spinning rates was improper. To take care of this, we used the 5 pulse PASS method, and measured new sideband intensities at a much slower spinning rate of 2000 Hz. As you can also see below, these parameters (which are somewhat different from those previously obtained, but are not presented here due to space limitations) yield corrections that are still wildly outside of the range that most people would consider reasonable for the slowest spinning rate.
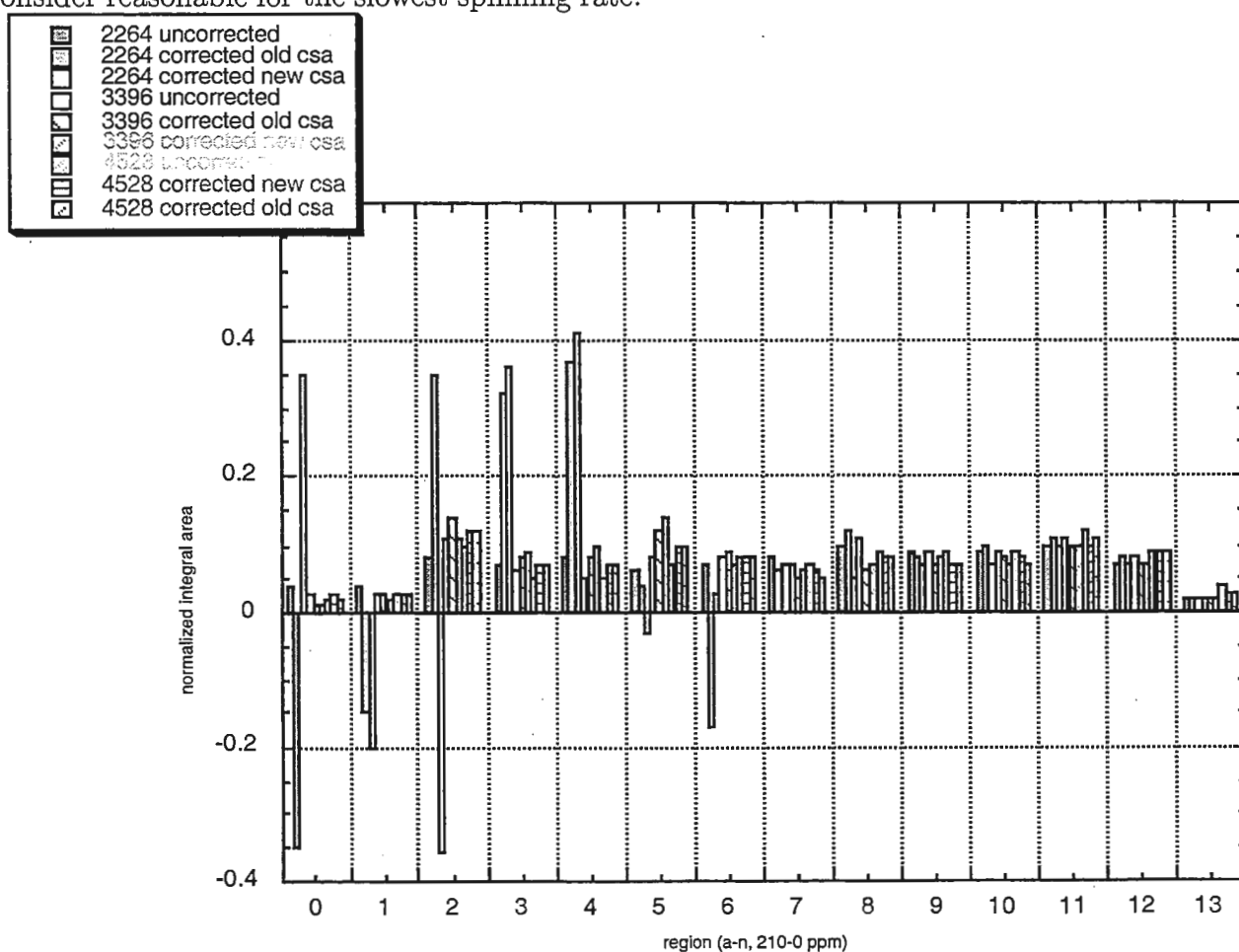
Perhaps it is not surprising that we cannot properly correct for sideband contributions in a series of spectra which have such similar integral areas across such a range of spinning rates. Because of the ill defined nature of these humic and fulvic acid spectra, it is possible that the method might work better on spectra that were more well defined; e.g. those of a polycrystalline sample. To test this we used anisic acid; which contains many of the same carbon types as humic and fulvic acids. Again, the 5 pulse PASS method was used to obtain the sideband

intensities and the Mathematica notebook *(5)* was used to fit the intensities to chemical shift parameters. In this case we also used published csa values for the aromatic carbons *(6)* to see if those yielded different results.
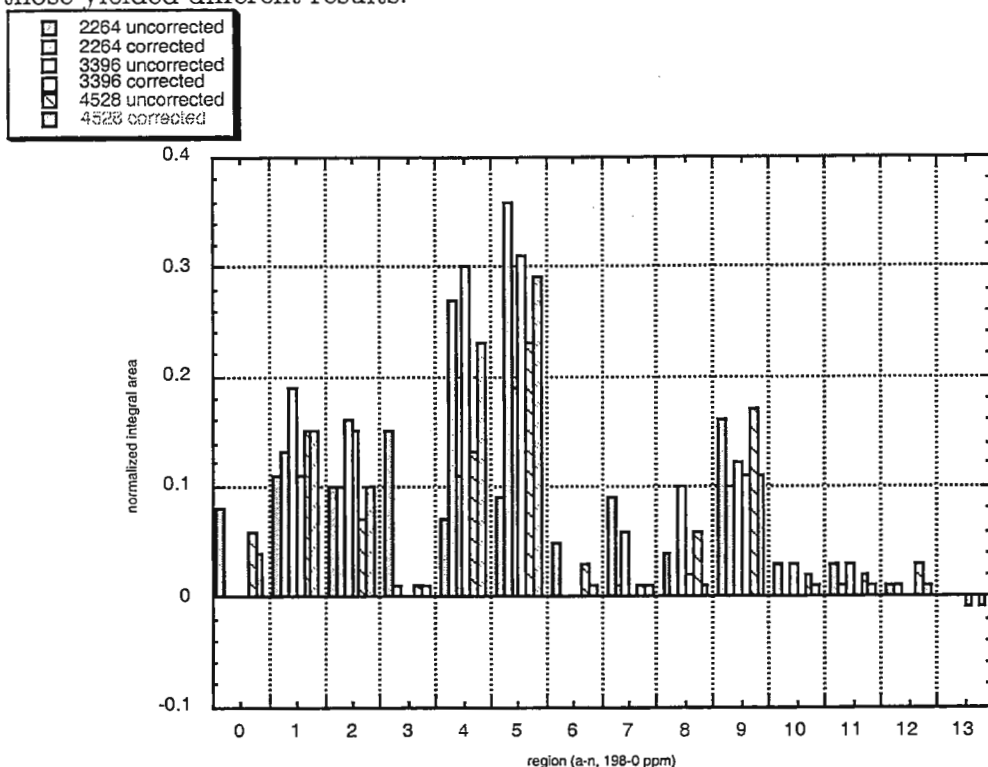
In this situation a reasonable correction is obtained at all spinning rates irrespective of which csa values we use, and the corrected data contain only positive intensities and only in those regions where intensity is expected (1,2,4,5 and 9).

There are potentially a couple of reasons for the poor performance of this method in the current application. First, the method may be unstable when applied to broad, poorly defined spectra such as those encountered in humic and fulvic acids, and this becomes particularly apparent when large corrections are applied. Second, the measured chemical shift parameters may be skewed toward carbon types which have a greater response in the experiment used (*e.g* those with longer T_2 s) and are thus not representative of the sample as a whole. Further investigation into these possibilities is underway.

References

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2. Randall, E.W., Mahieu, N. and Ivanova, G.I. (1997) "NMR Studies of soil, soil organic matter and nutrients: spectroscopy and imaging". *Geoderma*, **80**, 307-325.

3. Pratum, T.K. and Sletten, R.S. (1994) "^{13}C MAS Sideband Analysis and Correction in Humic and Fulvic Acids", Poster WP244, 35th ENC, Asilomar CA.

4. Feaux deLacroix S., Titman J.J., Hagemeyer A. and Spiess H.W. (1992) "Increased resolution in MAS NMR spectra by two dimensional separation of sidebands by order". *J. Magn. Reson.* **97**, 435-443.

5. O. N. Antzutkin, Y. K. Lee and M. H. Levitt (1998) "13C and 15N Chemical Shift Anisotropy of Ampicillin and Penicillin-V studied by 2D-PASS and CP/MASS NMR," *J. Magn. Reson.* **135**, 144.

6. Morgan K.R. and Newman R.H. (1990) "Principle values of carbon-13 NMR chemical shift tensors for a collection of substituted benzenes". *J. Am. Chem. Soc.* **112**, 4-7.

3

SEARLE

Dr. Bernard L. Shapiro
966 Elsinor Court
Palo Alto, CA 94303

September 1, Y2k-1
(received 9/4/Y1K+999)

Liquid Nitrogen Level Indicator

Dear Barry,

A method of measuring the level of Liquid Nitrogen in a cryostat is sometimes done by immersing a wooden dowel rod in the Liquid Nitrogen, and then waving it in the air after removal from the cryostat. The level of LN2 is then indicated by moisture, in the form of frost, building up on the cold portion of the dowel rod. I, however, have not mastered this art.

A much more precise and faster way to make this measurement is by using a non-magnetic metal tube (I use aluminum) which is terminated in a pneumatic switch *. (The switch has a specified sensitivity of 0.6 inches of water.) I used LED's (light emitting diodes) as visual indicators. Two LED's are wired in series with the normally open contacts of the switch and a 1000 ohm resistor. A 9 volt battery is used to power the device. When the open end of the tube is immersed in the LN2, both LED's will light. I placed one LED on the side of its box, and the other LED on the bottom. It has been my experience that the measurement precision of this technique is 4 mm.
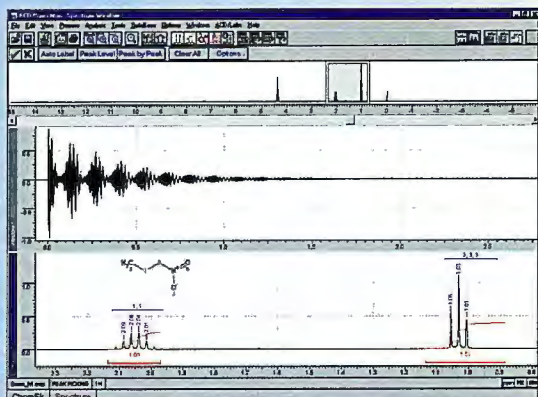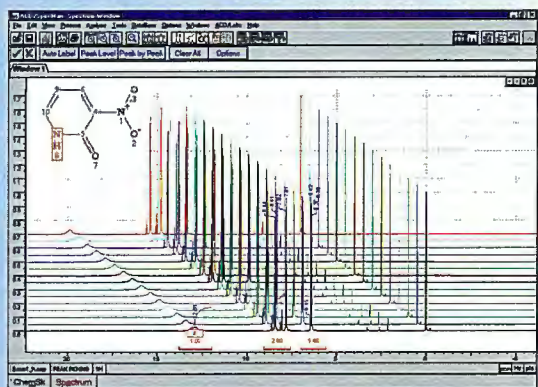
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Robert Dykstra

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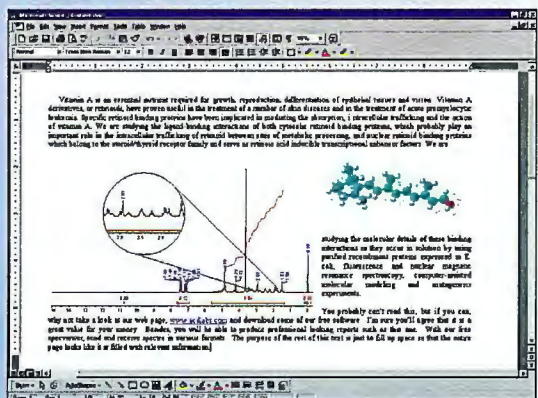 Fort Lauderdale, FLn33309

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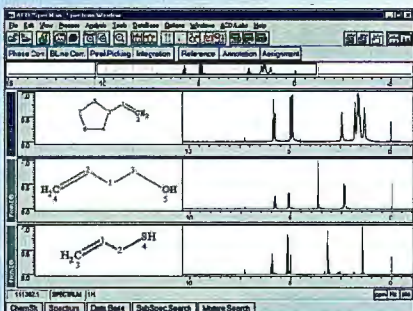Toll Free: 1-800-304-3988
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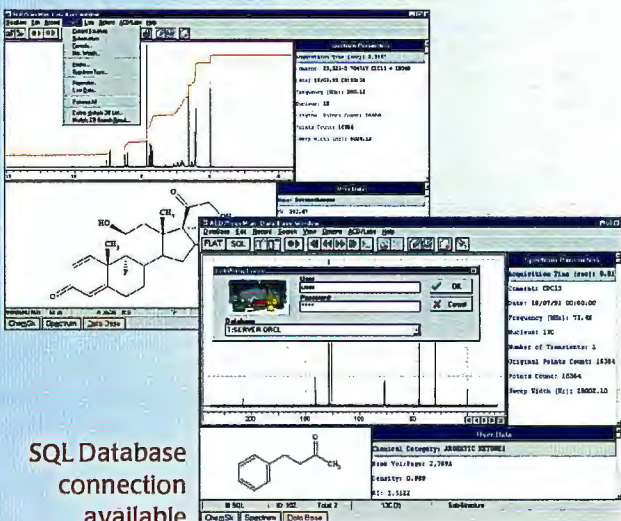www.acdlabs.com
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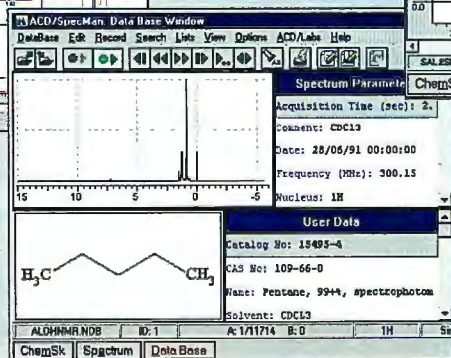
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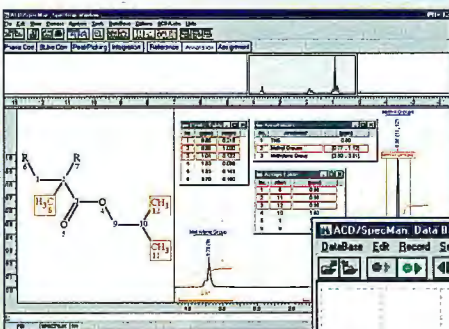
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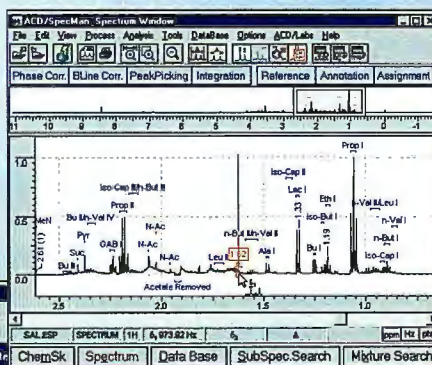
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SMASH

Small Molecule NMR Conference
Argonne National Laboratories
Argonne, Illinois
August 15-18, 1999

September 8, 1999

Bernard L. Shapiro, Ph.D.
Editor, The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

SMASH '99

Dear Barry,

As a follow-up to an announcement you published in The NMR Newsletter some months ago announcing the SMASH '99 Small Molecule NMR Meeting we thought it appropriate to share with the readership the outcome of the meeting.
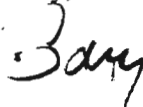
Participation was significantly greater than the organizing committee had originally hoped. Final registration was a total of 174 scientists, with ~20% from outside of the US. The meeting was held from August 15-18 at the Argonne National Laboratory conference center outside of Chicago. Jim Shoolery, formerly of Varian NMR, gave the plenary introductory lecture Sunday night entitled "From Neat Liquids to Nanograms." The Monday evening lecture, "A Tale of One Small Molecule," was given by Ray Freeman, and Tom Farrar rounded out the after dinner program on Tuesday night with a lecture entitled "Antediluvian Anecdotes of Sensitivity Enhancement Advances in NMR Spectroscopy." All three of the lectures from this well-known trio of NMR scientists were superb; the organizing committee would again like to thank Varian and ACD Laboratories for their sponsorship of the plenary lecturers.

The scientific program began Monday morning with sessions on Natural Products NMR followed by a session on Pulse Sequences. After an open session to allow attendees to interact or tour the Argonne National Laboratory's Advanced Photo Source. There was a late afternoon session on New Probe and Magnet Developments followed by dinner and Ray Freeman's plenary lecture. Tuesday's scientific program began with a session devoted to Application of Flow NMR followed by a session on Metabolism. Tuesday afternoon provided a second open session for the exchange of techniques and ideas amongst participants and another opportunity for interested scientists to tour the Advanced Photo Source. The late afternoon session on Tuesday was Applications of NMR to High Throughput Screening and Combinatorial Chemistry. Tom Farrar gave the Tuesday after dinner lecture, which was humorously delayed for a few minutes by the need to "shim" the overhead projector – accomplished by vigorous application of the butt of a maintenance man's hand to the projector! A Poster session followed on Tuesday night, with refreshments generously provided by Bruker Instruments. The final session of the meeting was held Wednesday morning and dealt with Post-Acquisition Data Processing, Databasing, and Spectral Prediction.

During the meeting, the Organizing Committee discussed the prospects for SMASH *2000*. Based on the very heavily positive feedback on the organization and content of this year's meeting, it was decided to hold SMASH *2000* at the Argonne National Laboratory Conference Center again next year. Next year's meeting will be held July 16-19, 2000. The organizing committee discussed session topics and potential session chairs for next year's meeting. Details of the planned sessions and their respective chairs follow in this issue of The NMR Newsletter and will also be available in a few weeks on the web at www.smashnmr.org. From the perspective of the Organizing Committee, SMASH '99 was a huge success! Attendance at this year's meeting clearly underscored the need for a meeting and forum devoted to scientists working in the area of small molecule NMR.

On behalf of the attendees and the Organizing Committee, SMASH '99, we would again like to thank the meeting's sponsors whose backing and confidence in the goals of the SMASH meeting are greatly appreciated. Sponsors included the following: ACD (Advanced Chemistry Development, Inc.), Bruker Instruments, Cambridge Isotope Laboratories, Isotec, Nalorac Corporation, Schering-Plough, and Varian, Inc.

Sincerely,

Gary Martin for the SMASH '99
Organizing Committee

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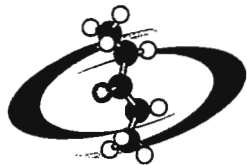
Improved Baseline Correction of FT NMR Spectra

September 10th 1999
(received 9/10/99)

Dear Barry,

As we all know, baseline correction can be a very essential step to obtain a high quality NMR spectra in some cases. Rolling baselines can make it difficult to identify peaks, as well as introduce a significant error into any quantitative measurements. The most convenient way of correcting baseline distortion is to construct a model of the baseline in the frequency domain and subtract it from the spectrum [1]. To this end, the majority of NMR desktop software allow the user to manually set the points belonging to the baseline and interpolate between them using analytical functions to model the baseline completely. While the results can often be good enough the method requires manual intervention and cannot be used for batch processing. On the other hand, the quality of automatic procedures is rarely sufficient when the baseline has severe distortions. The failures are generally due to both inadequate types of analytical functions used for modeling and the poor recognition of the baseline.

We have recently developed a new method for baseline correction which is governed by two easily adjustable parameters. The essence of the method is attributed to two parts: baseline modeling and baseline recognition.

It is a natural desire for visual inspection to have the baseline be a flat straight line with no constant offset. Our idea is to use the smoothed spectrum to model the baseline. We have used an averaging of neighboring data points of the spectrum, an operation equivalent to convolution with a rectangular function. The number N of points to average, or the width of the rectangle, is the first parameter of our procedure. It is evident that subtraction of the smoothed spectrum from the original one can give a relatively flat straight line, but it makes sense only for the area that does not contain peaks. As a result we have a fragmented model, which needs interpolation over the area where peaks are present. Interpolation can be as simple as connection by straight lines, or as complicated as we care to make it. The second important point is recognition of the baseline separately from the peaks.

Since the ultimate definition of "baseline" is "not containing peaks" it is natural to employ for its recognition the same tool that is used for peak identification. We have developed the following procedure. To decide whether the *i-th* point belongs to the baseline it is placed in the center of a rectangle with a width of N spectral points. Among these N points the minimal and maximal values are found. If their difference does not exceed the noise standard deviation multiplied by a definite factor (the second parameter of our technique) the *i-th* point is considered to belong to baseline. Finally the baseline model is then subtracted from the spectra.

Figures 1 and 2 below illustrate the results obtained with our approach. A characteristic rolling baseline can be observed in the spectrum in Figure 1 and can be accounted for by corruption of the first several points of FID. A well known algorithm was applied to this problem [2], and its performance is comparable with that of our method. However for the second case (Figure 2.) our approach gives a far superior result. Due to adequate baseline modeling and recognition our technique has been shown to be superior and therefore of inherent value for desktop post-processing.
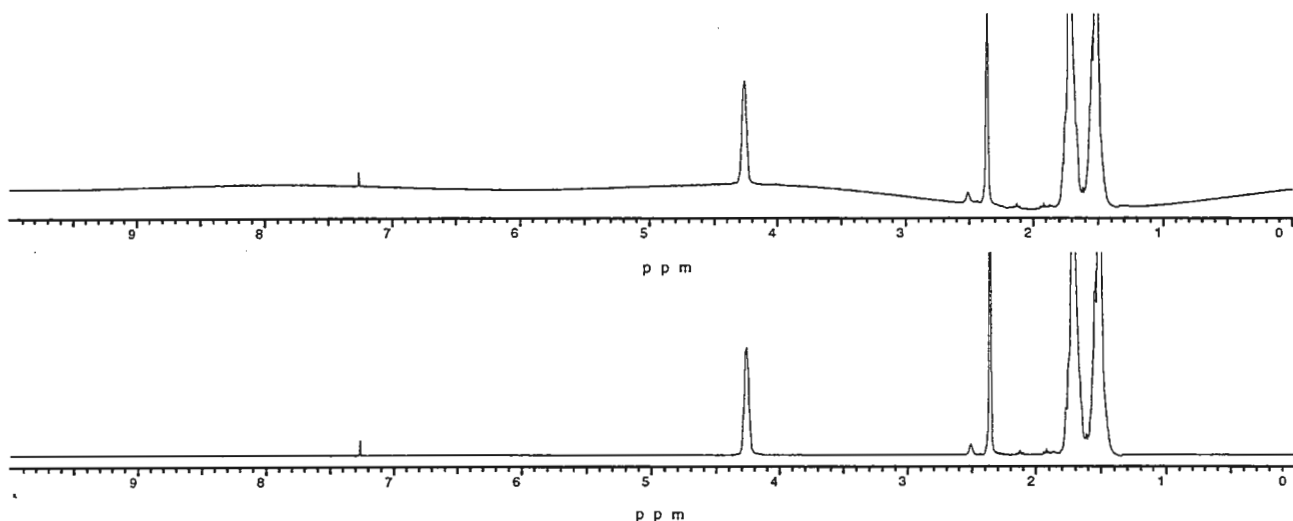
Figure 1. Original experimental (top) and baseline corrected (bottom) ^{1}H NMR spectra of cyclopentanol in CDCl$_3$. The rolling baseline is due to the first several points of the FID being corrupted.
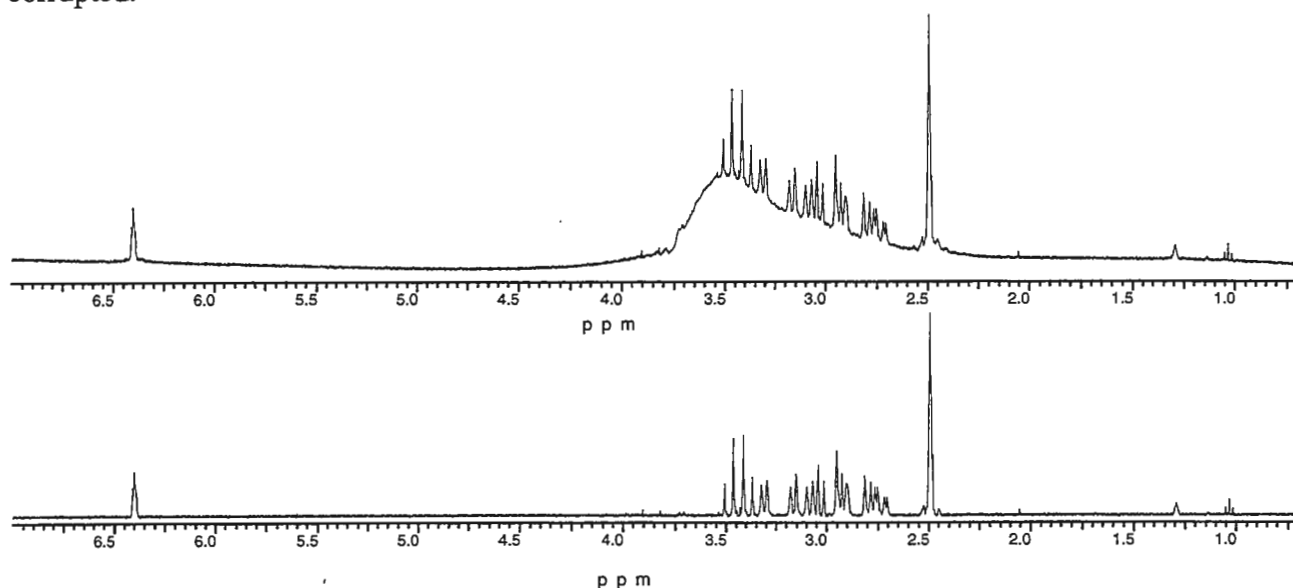
Figure 2. Original (top) and baseline corrected (bottom) ^{1}H NMR spectra of 6-bromo-1,5-dinitrobicyclo[3.3.1]non-6-ene-3-carboxylic acid in DMSO-D$_6$. The hump in the original spectrum is due to non-optimal water suppression.

Yours sincerely,

Sergey Golotvin and Antony Williams,
Advanced Chemistry Development

P.S. Your readers may wish to take advantage of the FREE NMR viewer now posted at our website (www.acdlabs.com/download). This includes an integrated Structure Drawing Package, Chemsketch.

References:

1. Hoch J.C. and Stern A.S.: NMR data processing, p. 196, New-York, 1996, Wiley-Liss.
2. Heuer A. and Haeberlen U., J.Magn.Reson. **85**, 79 (1989)

SMASH-*2000*

"Small Molecules Are Still Hot"
Small Molecule NMR Conference
July 16-19, 2000
Argonne National Laboratory
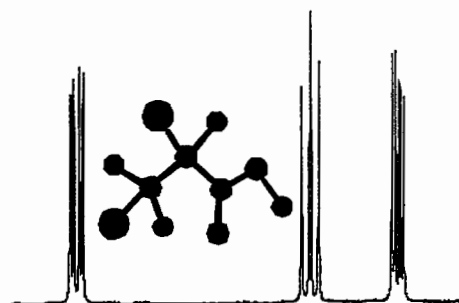. Conference Center, Chicago, Illinois

SMASH

G.E. Martin – Program Chairman

Tentative Schedule

Sunday, July 16	12:00-5:00	**Registration**	G. Nemeth, R. Espina, M. Levenberg, G. Chmurny
	6:00-7:00	**Plenary Speaker**	TBA
	7:00-10:00	**Dinner/Mixer**	
Monday, July 17	7:00-8:15	**Breakfast**	
	8:25-8:30	**Opening Remarks**	
	8:30-10:30	**Natural Products**	P.J. Sidebottom
	10:30-11:00	**Coffee Break**	
	11:00-12:30	**Pulse Sequences**	A.J. Shaka
	12:30-2:00	**Lunch**	
	2:00-3:30	**Graduate Student/ Post Doc Session**	R.T. Williamson
	3:30-5:00	**Break/Advanced Photon Source Tours**	
	5:00-7:00	**Dinner**	
	7:00-?	**Plenary Speaker**	TBA

Tuesday, July 18

Time	Session	
7:00-8:15	**Breakfast**	
8:30-10:30	**Metabolism**	J.P. Shockcor
10:30-10:30	**Coffee Break**	
11:00-12:30	**Small Molecule Solid NMR**	A.G. Swanson
12:30-2:00	**Lunch**	

2:00-5:00 **Free Afternoon, Advanced Photon Source Tours or Workshop Attendance**
Potential Workshops – individuals who have expressed interest in being involved

    Structure Elucidation – G. Chmurny, D.J. Russell
    LC/NMR – A. Swanson, S.R. Maple
    Metabolism NMR – J.P. Shockcor
    CombiChem/HTS – M. Shapiro, G. Nemeth
    FDM – A.J. Shaka

6:00-11:00 **Poster Session/Buffet Dinner in Poster Area**
    D. Lankin,
    Poster Session Co-ordinator

Wednesday, July 19

Time	Session	
7:00-8:15	**Breakfast**	
8:30-10:30	**Tips & Techniques** (8x15 min presentations)	D. Lankin
10:30-11:00	**Coffee Break**	
11:00-12:30	**Forensic NMR**	J. Myers & P. Hays Co-chairs
12:30-12:45	**Closing Remarks**	
12:45	**Box lunch & departure**	

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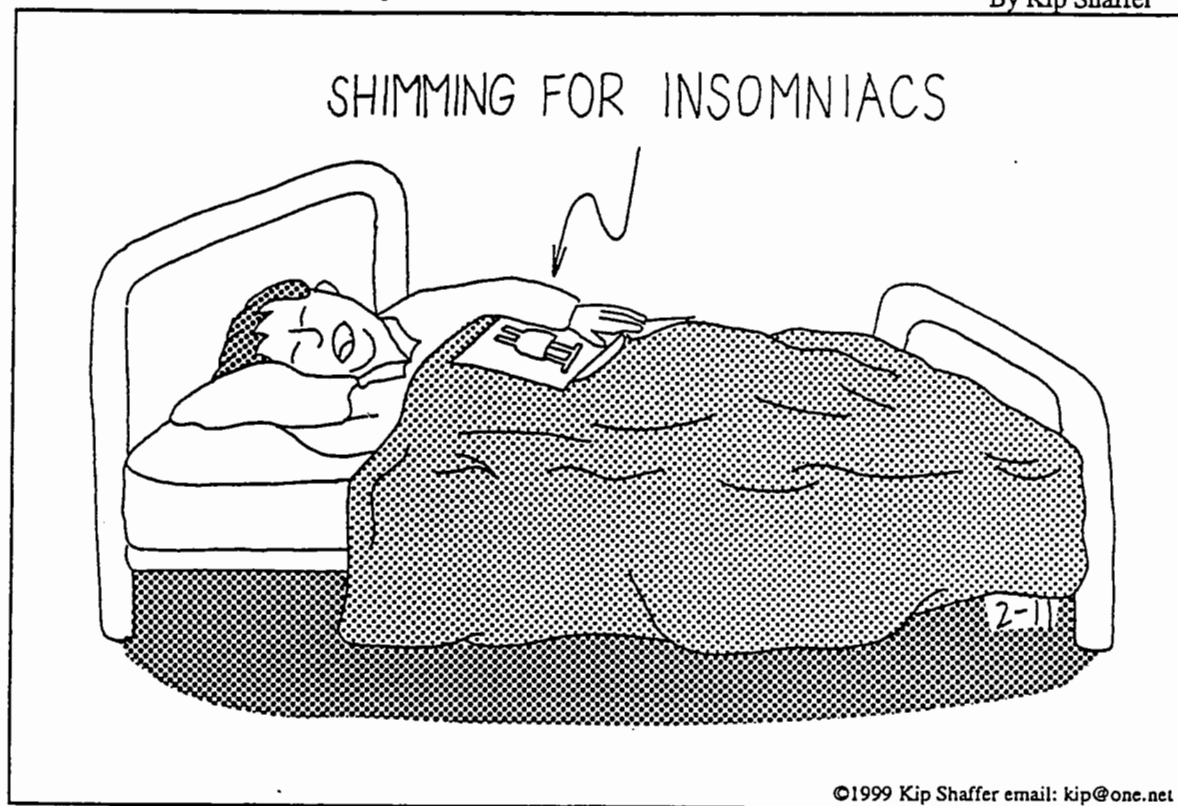
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Field of Dreams

By Kip Shaffer

SHIMMING FOR INSOMNIACS

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NEWSLETTER

Policies and Practical Considerations

The NMR Newsletter (formerly the **TAMU NMR Newsletter**, the **IIT NMR Newsletter**, and originally, the **Mellon Institute NMR Newsletter**), now in its forty-second year of consecutive monthly publication, continues under the same general policies as in the past.

1. Policy:

The 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. Technical contributions should always contain a significant amount of information that has not already been published or that will appear in the formal literature within a few weeks of the appearance in the Newsletter.

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'. The Newsletter is not, and will not become, a journal. We merely reproduce and disseminate exactly what is submitted.

2. Public Quotation and Referencing:

Reference to The NMR Newsletter by its present or previous names in the scientific literature is *never* permissible. Public quotation of Newsletter contents in print or in a formal talk at a meeting, etc., is expressly forbidden, except as follows. *In order to quote or use material from the Newsletter, it is necessary, in each individual case, to obtain the prior permission of the responsible author 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 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: Seven months after your last technical contribution, you will receive a "Reminder" notice. If no technical contribution is then forthcoming, nine 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, only one contributor may be credited. 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.

4. Finances:
The Newsletter is wholly self-supporting, and its funding depends on Advertising, Sponsorships, and individual Subscriptions. The **Subscription fee** for the October 1999 - September 2000 year is US$190, with a 50% academic or personal subscription discount. Subscriptions are available for a minimum of the twelve monthly issues which end with a September issue. However, a subscription can be initiated at any time, with the price for more than twelve issues being prorated.

Corporations are also invited to join 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 the Newsletter depends significantly on the generosity of our Sponsors, most of whom have been loyal supporters of this publication for many years. We will provide further details to anyone interested.

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 Newsletter will be included in the next issue if received on or before the published deadline dates.

b) Please provide short titles of all topics of your contributions, to ensure accuracy in the Table of Contents.

c) Contributions should be on 8.5 x 11" (21 x 27.5 cm) pages, *printed on one side only*. Contributions should be submitted in camera-ready condition. Contributions may not exceed three pages without prior approval. Each page must have margins of at least 0.5" (1.3cm) on all four edges. 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).

d) Please include your e-mail address on your contribution.

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.*

When formatting your contributions, please consider the following:

i) Try using a smaller type font: The body of this page is printed in 10 point type, which I believe is adequate for most purposes. Even 11 or 12 point type is acceptable if the particular font is not too large. Type smaller than 8 point should not be used.

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. 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.

6. **Suggestions**: They are always welcome.

October 1999

*Telephone: 650-493-5971. Please confine telephone calls to 8:00AM-10:00PM, *Pacific Coast Time.*
*Fax: 650-493-1348 (Do not use for technical contributions which are to appear in the Newsletter,
	for Fax quality is not adequate.)
*Email: shapiro@nmrnewsletter.com
*http://www.nmrnewsletter.com

Deadline Dates

No. 494 (Nov.)	22 Oct. 1999
No. 495 (Dec.)	26 Nov. 1999
No. 496 (Jan.)	24 Dec. 1999
No. 497 (Feb.)	21 Jan. 2000
No. 498 (Mar.)	25 Feb. 2000

Mailing Label Adornment: Is Your Dot Red ?

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