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A monthly collection of informal private letters from laboratories involved with NMR spectroscopy. Information contained herein is solely for the use of the reader. Quotation of material from the Newsletter is not permitted, except by direct arrangement with the author of the letter, in which case the material quoted must be referred to as a "Private Communication". Results, findings, and opinions appearing in the Newsletter are solely the responsibility of the author(s). Reference to The NMR Newsletter or its previous names in the open literature is strictly forbidden.

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- automatically measure integrals of preset regions
- output calculated values as text annotation on the spectrum

NEW! Buffers for displaying multiple spectra

Spectra displayed on the same ppm scale
even with unequal
- number of data points
- spectrometer frequency
- sweep width
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## FORTHCOMING NMR MEETINGS

- **NMR Spectroscopy of Polymers**, Breckenridge, Colorado, **January 24-27, 1999**; an International Symposium
  Sponsored by the Division of Polymer Chemistry, American Chemical Society; Organizers: P. T. Inglefield and A. D. English; Registration contact: Neta L. Byerly, Division of Polymer Chemistry, Inc., Virginia Tech, 201 Hancock Hall, M.C. 0257, Blacksburg, VA 24061; 540-231-3029; Fax: 540-231-9452; email: nbyerly@vt.edu.

- **7th Annual “Advances in NMR Applications” Symposium**, Omni Rosen Hotel, Orlando, Florida, **February 28, 1999**; Contact: Kathy Bishop, at the Nalorac Corp.; 510-229-3501; kathy.bishop@nalorac.com; See Newsletter 484, 30.

- **40th ENC (Experimental NMR Conference)**, Clarion Plaza Hotel, Orlando, Florida, **February 28 - March 5, 1999**, immediately preceding Pittcon in Orlando; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87505; (505) 989-4572; Fax: (505) 989-1073; Email: enc@enc-conference.org.

- **Pittcon ‘99**, Orlando, FL, **March 7-12, 1999** (50th year celebration of the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy.) Contact: The Pittsburgh Conference, Dept. CFP, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235-5503; 412-825-3220; Fax: 412-825-3224; e-mail: pittconinfo@pittcon.org.

- **Spin Choreography - a symposium in appreciation of Ray Freeman**, Cambridge, England, **April 8-11, 1999**; web site: [http://mchsg4.ch.man.ac.uk/mcmr/RF.html](http://mchsg4.ch.man.ac.uk/mcmr/RF.html); fax: c/o M.H. Levitt +46-8-15 2187; email: mhl@physc.su.se.

- **Seventh Scientific Meeting and Exhibition of the Intl. Soc. for Magnetic Resonance in Medicine (ISMRM)**, Philadelphia, PA, **May 22 - 28, 1999***; Contact: International Society for Magnetic Resonance in Medicine, 2118 Milvia St., Suite 201, Berkeley, CA 94704.

- **International School of Structural Biology and Magnetic Resonance**, 4th Course: Dynamics, Structure and Function of Biological Macromolecules; Erice, Sicily, Italy; **May 25-June 5, 1999**; Contact: Ms. Robin Holbrook, Stanford Magnetic Resonance Laboratory, Stanford University, Stanford, CA 94305-5055; (650) 723-6270; Fax: (650) 723-2253; Email: reh@stanford.edu. See Newsletter 483, 8.

*continued on p. 18*
Superimposing TROSY and anti-TROSY

Dear Barry:

A subject of great current interest in the biomolecular NMR community is TROSY introduced by Pervushin et al. (PNAS 94, 12366 (1997)). Here at Carlsberg we have been working on different ideas around TROSY. A paper with a new pulse sequence doing the same as earlier versions but with improved pulse economy is due to appear very soon in a Richard Ernst honorary issue of Molecular Physics. Something else that intrigued us right from the beginning is that TROSY does a fine job of selecting the peak of highest intensity but it also eliminates the rest of the cross peak components. That leads to the thought that it might be possible to put the eliminated coherence or spin order to good use.

What it amounts to is finding a way of suppressing heteronuclear one-bond coupling constants in indirect dimensions of multidimensional experiments. In other words, the low-frequency component must be shifted by \(|J|/2\) while the high-frequency component must be shifted by \(-|J|/2\). That is possible using the novel technique of TIG-BIRD (JMR 135, 44 (1998)) that allows arbitrary and independent manipulations of the two magnetizations of a doublet. Hence the solution is Spin-State-Selective Time-Proportional Phase Incrementation (S³ TPPI), i.e. to apply different TPPIs on the two components so as to achieve the desired shifts in frequency. This is what we have been working on most recently in a joint project with Jacques Briand.

We want to share with you some preliminary results of comparing TROSY with a new experiment combining TIG-BIRD with the standard gradient version of HSQC. Currently, the comparison between S³ TPPI HSQC and HSQC is not satisfactory. The results are obtained on a Bruker DRX 600 MHz spectrometer using a protein of MW about 20 kDa (NCAM modules 1 and 2, courtesy of Flemming M. Poulsen). F₂ sections from the ¹⁵N-¹H TROSY spectrum are to the right and the corresponding ones from the S³ TPPI HSQC spectrum (TROSY and anti-TROSY peaks superimposed) to the left.

Sincerely yours,

Ole W. Sørensen

Axel Meissner

Thomas Schulte-Herbrüggen
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- NMR-Check (diagnostic software).
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Q: Can NMR Suite for Windows NT control the spectrometer?
A: Yes! NMR Suite for Windows NT running on a PC has full control of the spectrometer and also does the data processing and data manipulation.

Q: Can I import spectra generated in NMR Suite for Windows NT into Windows programs such as MS Word or MS PowerPoint?
A: Yes! Our programs can write the plots into the Windows Clipboard or into a Windows Enhanced Metafile. From there the files can be imported into Word, PowerPoint and other Windows programs.

Q: Does NMR Suite for Windows NT replace NMR Suite running on the Silicon Graphics computers?
A: No! Bruker continues to support the SGI/IRIX platform. NMR Suite for Windows NT is an option, and the choice is yours!

Q: Is special hardware required for the PC to control the spectrometer?
A: No! The PC is connected to the spectrometer by a standard ETHERNET card. We require a second ETHERNET card to connect the PC to the INTERNET/INTRANET.

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- CD ROM
- 3 button mouse for PS/2 port
- Keyboard
- 2 ETHERNET cards, 10/100 Mbit 3COM 3C905 PCI bulk
- Windows NT 4.0 workstation installed on NTFS file system, including service pack 3

For complete details contact your local Bruker sales representative. We’d like to hear from you.

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Diffusion and peptide proton exchange

The work outlined here follows an idea from John Lindon. We have recently used $^1$H diffusion experiments to monitor peptide proton (NH) exchange in the cyclic peptide viomycin (see below). The experiment used was the 1-D longitudinal eddy-current delay (LED) modification of the pulse field gradient spin-echo experiment, incorporating WATERGATE and bipolar gradients to further reduce the eddy-currents. For non-exchanging protons the signal intensity follows a single exponential:

$$I_i = I_{0i} \exp(-K^2D\Delta)$$

where $K = \gamma G\delta$; $\gamma$ is the gyromagnetoc ratio, $G$ and $\delta$ are the strength and duration of the gradient, $D$ is the diffusion coefficient and $\Delta$ is the diffusion period. For intermediate rates of exchange - when the residence time ($t_p$) of the labile proton on the peptide is less than, but not a lot less than $\Delta$, the signal intensity follows a more complicated function, and following Moonen et al. we derived:

$$I_i = I(E)_{0i} \exp\{[-K^2(D_wf_w + D_pf_p)\Delta]\} + I(N)_{0i} \exp\{-K^2D_p\Delta\}$$

where $I(E)$ and $I(N)$ are constants, $f_p$ and $f_w$ are the fractions of the diffusion period that the proton spends on the peptide and water respectively ($f_w = 1 - f_p$) and $D_w$ and $D_p$ are the diffusion coefficients of water and the peptide respectively. We determine $D_p$ from the resonances of non-exchanging protons and $D_w$ from a separate experiment without WATERGATE. A double exponential fit of the $I_i$ data for the NH protons then gives values for $f_p$ then $t_p = f_p\Delta$, and the pseudo first order rate coefficient for the exchange may be estimated as $t_p^{-1}$.

We have tested the validity of the method by comparing the rate coefficients we obtained from this experiment with those obtained some time ago in Chris Dobson's group (see attached graph) using 2-D magnetisation transfer (NOESY). Our measurements were made on a sample at pH = 5.6 while the published data were from a sample at pH = 4.2 - much slower exchange. The correlation is good, but another important feature is that the 'diffusion' method clearly can determine much faster rates than the NOESY (EXCSY) method, which seems to have an upper limit around 5 to 10 s$^{-1}$. 


Viomycin Exchange Rates /s⁻¹

All credit to John Lindon and Jeremy Nicholson for this, which is now accepted for publication.⁸

Best wishes.

---

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TIG-BIRD: Arbitrary and Independent Manipulations of $I$, $IS^a$ and $IS^b$ Spin Systems

Dear Barry:

Recently we have described our new pulse sequence element dubbed TIG-BIRD (Triselective Independent Gyrations BIRD) (J. Magn. Reson. 135, 44-49, 1998) for simultaneous and independent rotations with arbitrary flip angles and phases for isolated $I$, $IS^a$ and $IS^b$ resonances without the use of selective radiofrequency pulses. TIG-BIRD generalizes earlier pulse sequence elements like BIRD, TANGO, BANGO, and BIG-BIRD, the latter of which allows for arbitrary selection of flip angles and phases for $I$ and $IS$ spin systems without discriminating between $IS^a$ and $IS^b$ resonances. TIG-BIRD also generalizes the Spin-State-Selective ($S^3E$) element which can selectively excite only one of the $IS^a$ and $IS^b$ resonances.

When isolated $I$ spin systems are irrelevant, $\alpha,\beta$ TIG-BIRD is a four-pulse sequence element, as shown in Figure 1a, for arbitrary and independent manipulations of $IS^a$ and $IS^b$ resonances. When isolated $I$ spin systems do also need to be considered, the full TIG-BIRD pulse sequence, as shown in Figure 1b is used. The full TIG-BIRD can be considered as a combination of BIG-BIRD and $\alpha,\beta$ TIG-BIRD. The flip angles and phases of the rf pulses on the proton channel are calculated in such a way that the cumulative effect of the pulse sequence element generates the desired flip angles and phases for $I$, $IS^a$ and $IS^b$ resonances:

$$
\begin{align*}
I : & \left(\frac{\pi}{2}, \phi \right)
IS^a : & \left(\frac{\pi}{2}, \phi \right)
IS^b : & \left(\frac{\pi}{2}, \phi \right)
\end{align*}
$$

Figure 1
Figure 2 illustrates the enhanced capability obtained with TIG-BIRD in being able to arbitrarily and independently vary the phases and flip angles for the three resonances. A series of one-dimensional spectra was recorded for different combinations of desired flip angles ($\gamma$, $\gamma'$, $\gamma''$) and phases ($\phi'$, $\phi''$, $\phi'''$) for $I$, $I_{S}^{\alpha}$ and $I_{S}^{\beta}$ resonances, respectively. These spectra were recorded on a sample containing 1% iodomethane with about 60% $^{13}$C-labeling in CDCl$_3$. All spectra were phase-corrected with the same zero- and first-order phase corrections and plotted with the same scaling factor.

![Figure 2](image)

We are currently evaluating applications that could exploit this new feature.

Sincerely yours,

Jacques Briand & Ole W. Sørensen (Carlsberg Laboratory, DK-2500 Valby, Denmark)
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Title: $^{19}$F NMR of Metabolites of Trifluoperazine in Rat Brain

Also: NEW PHONE NUMBERS

Dear Barry:

Fluorine-containing, psychoactive drugs have been studied in vivo in both human subjects and animal models using $^{19}$F NMR spectroscopy. The drugs, which typically contain a trifluoromethyl group, usually yield a single $^{19}$F resonance in vivo. However, a psychoactive drug is often metabolized in brain and other tissues to a variety of compounds, which themselves may have therapeutic or toxic activity. It would be valuable to observe these compounds independently in vivo. The relatively large line widths encountered in vivo usually preclude observation of separate resonances for primary metabolites because their molecular structure is often very similar to the drug itself.

With Sabine Strohschein, Ursula Breyer-Pfaff, and Klaus Albert of the University of Tübingen, Roger M. Hawk of the University of Arkansas at Little Rock, and Craig N. Karson of the Little Rock VA Hospital, we have studied the $^{19}$F in vivo NMR spectra of the heads of rats given the antipsychotic drug trifluoperazine (TFP). Resonances from unidentified metabolites were observed at about -57 and -75 ppm from CC$_3$F in a number of spectra, in addition to the primary peak at about -62 ppm. Tissue extracts were studied to confirm metabolite contributions to the in vivo spectra. Contributions to the spectrum from tissues other than brain were shown to be minimal. Although the -57 ppm metabolite was not confirmed in any extract, the resonance at about -75 ppm was confirmed in brain and muscle. Several previously identified TFP metabolites were found to contribute to the primary in vivo $^{19}$F resonance at about -62 ppm for rat head. The Figure on the next page shows the $^{19}$F spectrum from rat brain with some assignments, confirmed by spiking, and the corresponding molecular structures.

We also wanted to alert you to our new phone numbers, which are given above.

With best regards,

Richard A. Komoroski

Diana Lindquist
Trifluoperazine (TFP)
7-Hydroxytrifluoperazine (CF$_3$-OH)
Desmethytrifluoperazine (CF$_3$-PPP)

N-[y-(2-trifluoromethyl)phenothiazin-10-yl)-propylamine (CF$_3$-PPA)
Trifluoperazine sulfoxide (CF$_3$-SO)
N-[y-(2-trifluoromethyl)phenothiazin-10-yl)-propyl]ethylenediamine (CF$_3$-PPED)
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In a continuation of our work using $^{129}$Xe NMR to probe polymer morphology we have revived a long time interest in Poly (2, 6 - dimethyl - 1, 4 - phenylene oxide) (PXE). Depending on the method of preparation highly porous forms of PXE can be prepared. At low temperatures (ca -90° C) two peaks are observed for the $^{129}$Xe sorbed in the polymer. These resonances are centered around 180 ppm from the free gas resonance, and can be ascribed to different sorption sites or different pore sizes in the PXE.

2D NOESY shows exchange of the xenon between the two resonances. Exchange is produced by translational diffusion between the two environments; and the exchange process is spread over at least four decades in time indicating a broad distribution of time constants associated with this diffusion based process. The broad distribution of time constants for exchange could arise either from a distribution of length scales or a distribution of local diffusion constants. Note that the exchange starts in the two-dimensional pattern with a broadening in the middle of the shift range and only at very long times and high temperatures is exchange between all environments detected. Remembering that low shift values correspond to lower density regions and high shift values correspond to more dense regions, it appears that exchange begins by movement of the xenon gas between regions of only modestly different densities. This would account for the thickening of the two-dimensional pattern in the mid range of shifts. Exchange between regions of significantly different densities is observed only after long periods of time at high temperature.

These results argue that there is a spatial pathway where the gas diffuses from a low density region through an intermediate density region and then on to a higher density region. Jumps directly from a high density region to a low density region are not observed. This information is indicative of the kind of insights on local processes available from NMR.

Sincerely,

Paul T. Inglefield

Yingzi Wang
2D $^{129}$Xe NOESY as a Function of Temperature and Mix Time

Forthcoming NMR Meetings, continued from page 1:

Royal Society of Chemistry: 14th International Meeting on NMR Spectroscopy, Edinburgh, Scotland, June 27 - July 3, 1999; Contact: '99NMR14' c/o Mrs. Paula Whelan, The Royal Society of Chemistry, Burlington House, London W1V 0BN, England; +44 0171 440 3316; Email: conferences@rsc.org

SMASH No. 1 (Small Molecules Are Still Hot), Argonne, IL, August 15-18, 1999; Contact: Ms. Karen McCune, mccune_karen_e@lilly.com, 317-276-9783 or S. R. Maple, maple_steven_r@lilly.com or G. E. Martin, gary.e.martin@am.pnu.com or A. G. Swanson, alistair_swanson@sandwich.pfizer.com. See Newsletter 484, 29

"Applications of NMR to Complex Systems", Symposium at the American Chemical Society Meeting, New Orleans, LA, August 22-26, 1999; Contact: R. E. Botto, Symposium Chair, Chemistry Division, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439; 630-252-3524; Fax: 630-252-9288; E-mail: robert_botto@qmgate.anl.gov

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.

Additional listings of meetings, etc., are invited.
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- Conventional operation at the standard liquid helium temperature of 4.2 Kelvin
- Pumped (2.2K) operation, from the manufacturers' who developed this technology more than 25 years ago and refined it to produce the most reliable systems available today.

The manufacturers' who provide the most compact system available today, offering:

- Optimum transportability
- Ease of installation
- Minimum operational ceiling height

Engineering excellence available only from Oxford Instruments - setting the pace while others follow...
### Specifications for Vertical Bore, High Resolution NMR Magnet Systems

<table>
<thead>
<tr>
<th>NMR Operating Frequency (MHz/Hz)</th>
<th>200</th>
<th>300</th>
<th>400</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Field Strength (Tesla)</td>
<td>4.7</td>
<td>7.0</td>
<td>9.4</td>
<td>11.7</td>
</tr>
<tr>
<td>Nominal Room Temperature Bore Access (mm)</td>
<td>54</td>
<td>89</td>
<td>54</td>
<td>89</td>
</tr>
</tbody>
</table>

#### Magnet Types
- Standard
- Actively Shielded

| Field Stability (Hz/hour) | <2 | <2 | <3 | <3 | <5 | <5 | <10 | <10 |

Axial 5 Gauss Stray Field Contour (Metres):
- 1.81
- 2.65
- 2.19
- 2.75
- 4.2
- 1.5
- 1.8
- 2.5

<table>
<thead>
<tr>
<th>Radial 5 Gauss Stray Field Contour (Metres)</th>
<th>1.42</th>
<th>2.0</th>
<th>1.7</th>
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</thead>
<tbody>
<tr>
<td>Axial Stray Field Contour (Metres)</td>
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<td>2.1</td>
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<tr>
<td>Radial Stray Field Contour (Metres)</td>
<td>1.4</td>
<td>1.7</td>
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#### Cryostat Types
- Compact
- T3

<table>
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<tr>
<th>Minimum Helium Refill Interval (Days)</th>
<th>80 235 203</th>
<th>80 235 203</th>
<th>14</th>
<th>340</th>
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</thead>
<tbody>
<tr>
<td>Cryostat Type</td>
<td>T3 T5F8L T7</td>
<td>T3 T5F8L T7</td>
<td>T6L</td>
<td>T8</td>
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</table>

<table>
<thead>
<tr>
<th>Minimum Nitrogen Refill Volume (Litres)</th>
<th>32 61 61 32 61</th>
<th>32 61 61 32 61</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum Nitrogen Refill Volume (Litres)</td>
<td>32 61 61 32 61</td>
<td>32 61 61 32 61</td>
</tr>
<tr>
<td>Minimum Operational Ceiling Height (Metres)</td>
<td>1.89 2.92 2.92 2.92 2.92</td>
<td>2.92 2.92 2.92 2.92 2.92</td>
</tr>
</tbody>
</table>

| System Weight (kg) Including Cryogen's | 120 315 391 | 120 315 391 | 80 235 183 | 80 235 183 |

#### Dimensions
- External Diameter: 54 mm
- Internal Diameter: 89 mm

#### Room Temperature Shim Specifications

<table>
<thead>
<tr>
<th>Shim Type (Model)</th>
<th>Number of Channels</th>
<th>Dimensions</th>
<th>External Diameter (Cryostat Bore Size)</th>
<th>Internal Diameter (NMR Probe Diameter)</th>
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<tr>
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<td>45 mm</td>
<td></td>
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<tr>
<td>18/3373</td>
<td>18</td>
<td>89 mm</td>
<td>73 mm</td>
<td></td>
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<tr>
<td>26/3373</td>
<td>26</td>
<td>89 mm</td>
<td>73 mm</td>
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<tr>
<td>26/3373</td>
<td>28</td>
<td>51 mm</td>
<td>40 mm</td>
<td></td>
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<tr>
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<td>51 mm</td>
<td>40 mm</td>
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<tr>
<td>36/3151</td>
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<td>51 mm</td>
<td></td>
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</tbody>
</table>

#### Contact Information
- **UK**
  - Oxford Instruments
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  - Old Station Way
  - Eynsham, Witney,
  - Oxon, OX8 1TL
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  - MS D177, Palo Alto,
  - CA 94304-1030,
  - USA
  - Tel: +1 650 813 9068
  - Fax: +1 650 813 9069
  - e-mail: oinmrwest@aol.com

High-Order Multiple Quantum Excitation in Solid State $^{13}$C NMR

Dear Barry:

By now, there are many solid state NMR techniques for investigating local structural features of complex molecules, such as specific internuclear distances or dihedral angles. These techniques generally depend on specific isotopic labeling, usually with pairs of $^{13}$C and/or $^{15}$N nuclei. Local structural measurements are particularly useful for testing specific structural models or predictions. Recent work on an HIV-related peptide/antibody complex by David P. Weliky et al., which will appear in *Nature Structural Biology* in the near future, provides a good example of the importance of these techniques in biological problems. This work is the first application of solid state NMR in a structural investigation of a peptide/protein complex.

In cases where no credible structural models are available, no localized region is of principal interest, and the overall structural organization is unknown, solid state NMR techniques that provide more long-range or global structural information are needed. Solid state multiple quantum spectroscopy, as originally developed over 15 years ago by Alex Pines' group and subsequently investigated and applied by Jeff Reimer, Karen Gleason, Bernie Gerstein, James Yesinowski, Al Garroway, Serge Lacelle, and others, may provide such information. As shown by these people and their colleagues, multiple quantum spectroscopy can be used to determine the number of spins in a coupled group, thereby providing useful structural information. We have recently
shown that the time-reversible multiple quantum excitation pulse sequences that have been employed in earlier $^1$H and $^{19}$F multiple quantum NMR experiments, where dipole-dipole couplings are large and chemical shifts are small, can be easily modified for $^{13}$C multiple quantum spectroscopy of dilutely-labeled organic systems and biopolymers, where dipole-dipole couplings are small and chemical shifts can be large. Examples of $^{13}$C multiple quantum excitation spectra, obtained at 9.4 T on a Chemagnetics Infinity spectrometer, are shown here. Multiple quantum coherences up to tenth order, corresponding to simultaneous flipping of ten $^{13}$C spins, are observed. $^{13}$C-$^{13}$C distances are roughly 4 Å. This work will appear soon in the *Journal of Chemical Physics*.

We can imagine many applications of $^{13}$C multiple quantum spectroscopy in structural studies of peptides and proteins. For example, one could introduce a single $^{13}$C label at each alanine (or other amino acid) in a protein of unknown structure. Multiple quantum measurements might then reveal the sizes and geometries of clusters of coupled $^{13}$C nuclei that are formed when the protein adopts its native secondary and tertiary structure. Information about $^{13}$C cluster sizes and geometries would place strong, long-range constraints on the global protein structure. As another example, multiple quantum spectroscopy could be used to investigate helix-coil transitions in helix-forming synthetic peptides. If one places a single $^{13}$C label at every third amino acid residue in a peptide, then the labels will form a coupled chain with 5-6 Å spacings when the peptide is fully α-helical. When the peptide is in an extended or random coil conformation, the spacings will be significantly larger, up to about 12 Å, and the labeled sites will be uncoupled. Multiple quantum excitation spectra may then be used to determine the lengths of helical segments, or the distribution of these lengths, under conditions where the peptide is only partially helical. This information is not available from more traditional measurements, such as circular dichroism.

Sincerely yours,

Rob Tycko

Oleg Antzutkin

phone: 301-402-8272
fax: 301-496-0825
e-mail: tycko@helix.nih.gov
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Probes for biomolecular applications are available for a wide range of magnetic field strengths, sample sizes, and in an array of RF configurations. Gradient probes are available in both single-axis (Z) and triple-axis (X,Y,Z) configurations.

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Triple Resonance Probes
The premier probes for biomolecular applications, triple resonance probes are available in $^1H\{^{13}C/^{15}N\}$ for analysis of proteins and $^1H\{^{13}C/^{31}P\}$ for nucleic acid applications in a variety of sample sizes.

Penta Probes
Designed for versatility in biomolecular applications, Penta probes are pre-tuned to allow decoupling of up to four different types of nuclei ($^{13}C$, $^{15}N$, $^{31}P$, $^2H$), important in combined protein/nucleic acid research applications.

Tunable Triple Probes
These versatile probes, with a third multifrequency tunable channel, are ideal when applications range from biomolecular to chemical, and are available in $^1H\{^{13}C/X\}$ and $^1H\{^{13}P/X\}$ configurations.

Indirect Detection Probes
Designed for inverse detection experiments, indirect detection probes have optimal proton sensitivity and capability for decoupling irradiation for a broadband frequency range.
A Probe for Deform Polymer Networks in NMR Experiments

Dear Dr. Shapiro,

We describe here a home-built NMR probe which is used to perform $^2$H NMR experiments of polymer networks under deformation. The important features of this probe for deforming the polymer networks is its simplicity, easy to build and accurate measurements of deformation. Rubber sample $s$ is driven through the RF coil and then turn down to vertical direction from both sides over the freely rotatable rollers $b$ and $b'$. Both ends of the sample are clamped tightly by the clamps $c$ and $c'$ (opposite to the $c$) respectively. These two clamps are fixed to the plate $e$.

A threaded rod $f$ goes freely through the plate $g$ and again it goes through the female threads in the plate $e$.

The top end of the rod $f$ is free to rotate and the bottom end of it is fixed to a lever $h$.

Suppose the distance between two threads of rod $f$ is $x$. When the lever $h$ is turned clockwise one round, the plate $e$ is moved vertically downward by an amount of $x$ (and vice versa). Since $c$ and $c'$ are fixed to $e$, the sample $s$ is extended from both sides by amounts of $x$. Therefore, one clockwise turn of the lever $h$ corresponds to $2x$ macroscopic deformation of the sample. Since the distance $x$ between two threads can be made in sub millimeter scales, the above described probe can be used as one of the accurate tools of deforming the rubber samples in NMR experiments. In our $^2$H NMR experiments we are using this probe and one example is shown.

P. Ekanayake  
Heike Menge  
M. Knørgen

Please credit this contribution to the subscription of Prof. H. Schneider, Department of Physics, Martin-Luther-University Halle Wittenberg, Halle/Saale, Germany.
Figure 4 A deuterium NMR spectrum obtained from a cis-1,4 polybutadiene network (Mn=6500g/mol) under deformation (deformation ratio is 2.0), using the above described probe.
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We bring to the table over 40 years of NMR tube manufacturing experience found nowhere else. As the world-leading manufacturer of NMR tubes, we are proud to introduce our most popular selling tubes to you. Look no further, you are sure to find the specific size and type that will meet your demanding needs.

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Don't risk damaging your probe by using inferior brand NMR tubes.

Run your samples with total confidence. Request WILMAD Brand NMR Tubes for your next experiment.

### Standard NMR Tubes

<table>
<thead>
<tr>
<th>Size</th>
<th>Product Number</th>
<th>MHz</th>
<th>Length</th>
<th>Wall Thickness</th>
<th>Concentricity</th>
<th>Camber</th>
<th>Each</th>
<th>Qty.</th>
<th>Bulk Each</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 mm</td>
<td>542-PP-7</td>
<td>New!</td>
<td>800*</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00010&quot;</td>
<td>0.00015&quot;</td>
<td>35.00</td>
<td>+100 32.50</td>
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**J. Young Valve NMR Tubes**

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<th>Bulk Each</th>
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**Bruker Microprobe Tube**

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<td>2.50 mm</td>
<td>30.40</td>
<td>27.35</td>
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We are pleased to announce August 15-18, 1999, as the dates for the Small Molecules Are Still Hot (SMASH) conference. The Argonne Guest House, located on the grounds of the Argonne National Laboratory, has been selected as the site for the inaugural meeting. The Guest House offers excellent meeting facilities and accommodations, in addition to being located in Chicago, IL, which provides an international gateway for many of our colleagues.

The tentative schedule of events is arrival on Sunday, August 15, 1999 followed by an evening mixer. The bulk of the conference will be held on Monday and Tuesday (August 16-17) and will conclude at noon on Wednesday, August 18, 1999. The Argonne Guest House will handle all accommodation reservations. Details on the types of accommodations, pricing, and the methods for making reservations will be available in January 1999.

We would like to solicit your immediate assistance in two ways. (1) Please respond via e-mail or telephone to Dr. Gene Mazzola (epm@vm.cfsan.fda.gov or em105@umail.umd.edu; 301-405-1826) with your intentions regarding this conference. Specifically we would like for you to indicate ONE of the following in your response:

(i) I will definitely attend the SMASH conference  
(ii) I may attend the SMASH conference  
(iii) I will not be attending the SMASH conference

Your immediate response to this request is very important in putting together a successful SMASH conference. (2) Please give careful consideration to the types of information you would like to see included in the program, whether or not you would like to share new developments in your laboratories, and which colleagues you would enjoy hearing from during the conference. Your comments and suggestions regarding the program should be sent to Ms. Karen McCune (mccune_karen_a@lilly.com and 317-276-9783) by no later than the end of January 1999.

Your participation in the SMASH conference is vital for its success. We encourage our industrial colleagues to consider a corporate financial contribution, and we would like to encourage you to spread the word of this conference to interested individuals in academia, industry, and government agencies.
ADVANCES IN NMR APPLICATIONS

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FEATURING THE LATEST DEVELOPMENTS IN EXPERIMENTAL TECHNIQUES
SUNDAY, FEBRUARY 28, 1999 1:00 TO 6:00 P.M.

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(LOCATED A SHORT WALK FROM THE CLARION PLAZA HOTEL)

Partial Agenda Includes:

METHODS FOR IMPROVING NMR STRUCTURE DETERMINATIONS OF RNA
Arthur Pardi, University of Colorado

PROGRESS IN AFFINITY NMR
Aidi Chen and Michael Shapiro, Novartis Institute for Biomedical Research

OH MY GOD, THEY SHRUNK THE SAMPLE
Gary Martin, Pharmacia & Upjohn, Inc.

LC-NMR-MS: IS THE INFORMATION WORTH THE INVESTMENT?!
Steven R. Maple, Andreas Kaerner, Craig A.J. Kemp, Edward G. Groleau, and Karen A. McCune,
Eli Lilly and Company

TRIPLE RESONANCE NMR: PRACTICAL CONSIDERATION OF $^{13}$C / $^{19}$F / $^1$H
EXPERIMENTS ON SMALL MOLECULES
Jim Beery, BASF Corporation

NEW PROBE TECHNOLOGY FOR AUTOMATED NMR
Claude Jones, Monsanto Company
Ron Crouch, Atholl Gibson, and Toby Zenis, Nalorac Corporation

FROM ALIGNMENT TO STRUCTURE IN HIGH RESOLUTION NMR
Nico Tjandra, National Institutes of Health

USE OF CHEMICAL SHIFT FOR DETERMINATION OF PROTEIN STRUCTURES
Gabriel Cornilescu, Frank Delaglio, and Ad Bax, National Institutes of Health

APPLICATIONS OF THE TROSY TECHNIQUE
Arthur G. Palmer and J. Patrick Loria, Columbia University
Mark Rance, University of Cincinnati

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<table>
<thead>
<tr>
<th>Task</th>
<th>Platform</th>
<th>Time</th>
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<tr>
<td>1D processing; 8K* → 128K* with automated baseline correction</td>
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<tr>
<td>2D processing; 512<em>256</em> → 1024x1024</td>
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<td>Sparc 10 (UNIX)</td>
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<tr>
<td>2D processing; 512<em>256</em> → 1024x1024 with automated baseline correction in both dimensions</td>
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<td>Amide-detected 3D processing scheme; 512<em>64</em>×252* with solvent filtering and one zero-fill in each dimension</td>
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<td></td>
<td>Sparc 10 (UNIX)</td>
<td>3292 sec</td>
</tr>
</tbody>
</table>

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Phase and Coherence Level Decoding - A New Computer Program

Dear Barry;

As we all know, vendors of NMR spectrometers supply with their software an entire battery of pulse sequences with phase cycles for coherence selection. Determining the pathway selection is extremely difficult in certain cases. We have devised a computer program, DECODE95, for extracting the coherence pathways and tested this program on a number of Bruker and Varian pulse sequences. In doing so we were surprised to find anomalies in the phase cycles for some of these standard pulse sequences. Some of your readers may be interested in our findings. In the Varian cosyps.c sequence for the TPPI implementation (phase=3), the pulse sequence is coded to select only one pathway which leads to, upon Fourier transformation, the well known phase twist problem. To correct the problem, replace the statement in the pulse sequence:

if ((iphase == 1) || (iphase == 2)) with: if (iphase > 0).

We also found a problem with the phase cycle for the Bruker DEPT.AU pulse program. If the carbon-13 180 degree pulse is imperfect, two extraneous pathways can give signals, and this can lead to possible phase anomalies in the final spectrum. The standard Bruker phase cycle allows these pathways to sneak through. The following phase cycle allows only the desired pathways.

H1 90 3 2 3 2 1 2 1 2 1 0 1 0 3 0 3 0
H1 180 2 1 0 3 3 2 1 0 0 3 2 1 1 0 3 2
H1 theta 3 0 3 0 1 0 1 0 1 2 1 2 3 2 3 2
C13 90 0 1 2 3 0 1 2 3 0 1 2 3 0 1 2 3
C13 180 3 3 1 1 0 2 2 0 3 3 1 1 0 2 2 0
Receiver 0 1 2 3 0 1 2 3 0 1 2 3 0 1 2 3

The computer program, DECODE95, runs on Windows 95/98 platforms, and reads Bruker AM and Varian Unity programs, generates a coherence transfer diagram (HPGL format file) and lists the full phase cycle. Copies of DECODE95 may be requested by e-mail to nmrlab@sunfun.chem.ualberta.ca and full details of the program are to be published in the December issue of Concepts in Magnetic Resonance. Please credit this contribution to Tom Nakashima’s account.

Sincerely,

Ted McClung

Jason Ollerenshaw
December 16, 1998
(received 12/26/98)

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

SUBJECT: 3D Triple Resonance NMR of Organic Mixtures

Dear Barry:

Although much of our recent work has involved NMR of polymers, we have recently found use for 3D NMR in characterizing complex mixtures of small molecules.

Silylation of vinyl cyclobexene leads to a 6 component mixture of stereo – and regio-isomers (Figure 1). The 600 MHz 1H, 13C and 29Si spectra (Figure 2) are very complex, making it impossible to do much more than say it is a complex mixture. Twelve separate resonances are resolved in the 29Si 1D spectrum, as expected for a 6-component mixture.

A 1H,13C,29Si 3D chemical shift correlation experiment similar to the HNCA experiment used by biochemists can disperse 1H-13C HSQC-type correlations into a third dimension based on the 29CSi chemical shifts of the atoms which are part of the same spin system. The experiment can be run in three ways, with Csi to provide H-C-Si fragments, with CSi to provide H-C-C-Si fragments, and with CSi to provide H-C-C-C-Si fragments (Figure 3). The combined information from the three experiments permits assignments of all the resonances and the complete structure determinations for all 6 components in the mixture.

Unlike the experiments done in biochemistry, all of these data were obtained without the benefit of isotopic labeling. The experiments each require 4-8 hours of spectrometer time (not for sensitivity, but to obtain a sufficient number of increments in each of the evolution times) and the use of pulsed field gradients for coherence selection.

For the past year, we have been preoccupied with the replacement of our 600 MHz spectrometer with a 750 MHz instrument and many new accessories. Hopefully, we will show you some results from that equipment in our next contribution.

Best regards,

THE UNIVERSITY OF AKRON
Peter L. Rinaldi
Professor of Chemistry
Director of the Molecular Spectroscopy Laboratory

Weixia Liu
Graduate Research Associate
The University of Akron

DUPONT AUTOMOTIVE
Laurine Galye
Joan Hansen
Leck Wiczek
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Let's face it – the first priority of NMR manufacturers is to sell new instruments. Providing post-installation service and support is secondary, and sometimes takes a back seat in favor of the final test and installation of new systems. And of course, the manufacturers rarely, if ever, train new engineers to support older models, so the number of engineers that are available to support them tends to decline over time.

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♦ GE QE-300, including dual $^1$H/$^{13}$C electronics, $^1$H/$^{13}$C switchable probe. $45,000.
♦ Varian VX4-300, including broadband electronics, $^1$H/$^{13}$C switchable probe. $58,000.

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Customer Direct or full Fully Remanufactured - either way we have a program to fit your needs. Just tell us what you want, and let us do the rest!
I have been meaning to write for the past seven years since I joined the faculty at the University of Toronto to get my subscription underway but I am just a bit behind! One of the primary research interests in my laboratory focuses on the development of NMR methods for the study of the structure and dynamics of high molecular weight proteins and protein complexes. This requires (a) the production of proteins with optimal labeling, such as $^{15}$N, $^{13}$C, $^2$H with protonation at key sites such as methyl groups and (b) the development of NMR methodology which exploits the labeling strategy employed. Our long term goal is to develop an approach facilitating the rapid generation of global folds of high molecular weight molecules (in the 50 kDa range). Obviously we record large numbers of data sets and having the right tools at our disposal for data processing is absolutely critical.

My initial experience with the development of data processing software for multidimensional NMR came when I was a post-doc in Ad Bax's laboratory. In those days everything was new (and exciting!) and we had to write our own processing software from scratch. Although the software that Dominique Marion and I wrote was usable and quite flexible, it quickly became apparent that large numbers of improvements were necessary. Fortunately for me (and for that matter the whole NMR community) Frank Delaglio joined Ad Bax's lab at the NIH in 1991 and began the process of writing processing software. The end result was the creation of an extremely elegant and very flexible program called NMRPipe for processing N-D data sets.

Processing begins with the conversion of data from the format stored on the spectrometer to NMRPipe format using a simple script. It inserts the number of points in each dimension, spectral widths, frequencies, carrier positions, axis labels and dimensionality of the data set in a header to be used by the program later. Subsequently the data can be processed without the bother of remembering the number of points and hence the size of the matrix that is necessary or will be necessary once zero filling, linear prediction, etc., are done. All of the standard processing tools are available (and more) including a number of post-acquisition water removal schemes, excellent baseline correction modules, as well as several linear prediction (and MEM) functions. Basically, the user writes a simple UNIX shell script, which takes the unprocessed data and 'flows' it through a pipeline of processing programs. Each pipeline corresponds to a particular function such as baseline correction, Fourier transformation or water suppression. Scripts are easily modified from one application to the next. Visualization routines are, of course, also available (called NMRDraw) so that one can study the effects of application of a particular window function prior to the actual data processing, for example. In my experience an average post-doc can master the essentials of the program to be able to process his/her data in about 15 minutes!

continued
An example from our own work on maltose binding protein (MBP, a 370-residue protein) will illustrate the power of the program. We have prepared [Val, Leu, Ile (61)]-methyl protonated $^{15}$N, $^{13}$C, 2H-labeled protein and Kevin Gardner assigned the backbone $^{15}$N, $^{13}$C$^\alpha$, HN and the sidechain $^{13}$C$^\beta$ and methyl ($^{13}$C, $^1$H) chemical shifts. Naturally we wanted to obtain as many NOEs as possible to define the global fold. Catherine Zwahlen developed a number of NOE experiments for measuring NOEs to methyl groups with high resolution, necessary in the case of MBP with 122 methyl groups. In one experiment designed in collaboration with Andy Byrd's group we measured the methyl-methyl NOEs by recording the $^{13}$C methyl chemical shift of the methyl from which the NOE originates together with the $^{13}$C and $^1$H chemical shifts of the destination methyl.

In order to squeeze out the last NOE from our data set, resolution is paramount and we employ a scheme in which linear prediction is carried out in both of the indirect detection dimensions. It is important, however, that linear prediction be performed on a data set in which two of the three dimensions are already processed in order to minimize the number of oscillators. This necessitates undoing a whole set of transformations in one of the dimensions and redoing them after linear prediction. Frank's program handles this in a completely straightforward manner by including 'inverse' commands which undo previous processing. The 3D methyl-methyl NOE dataset on MBP was thus processed with minimal user effort.

NMRPipe has many other features, including routines for peak picking, volume fitting, analysis of J-coupling, dipolar coupling, and relaxation data and software for the analysis of data for structure determination. The program is reasonably well documented. Frank should be congratulated in writing what I think is the processing system of choice. The software has made a big contribution to the research in my lab.

Sincerely yours,

Lewis E. Kay
Protein Engineering Centers of Excellence
Departments of Medical Genetics,
Biochemistry and Chemistry
University of Toronto
Toronto, ON M5S 1A8
Canada.

*(from the Software Review Editor) NMRPipe is available for free for Unix from LCP/NIDDK at NIH. Send an email for ftp access to Frank Delaglio (delaglio@speck.niddk.nih.gov). A commercial version for Windows-NT is available from Resonance Designs, Inc.) For additional information see the ad in this issue of the Newsletter, or see http://www.resdesigns.com.*
Glycine-1-^{13}C,^{15}N, >99 atom % ^{13}C, >99 atom % ^{15}N

L-Aspartic Acid-1-^{13}C,^{15}N, >99 atom % ^{13}C, >99 atom % ^{15}N

L-Leucine-1-^{13}C,^{15}N, >99 atom % ^{13}C, >99 atom % ^{15}N

Glycine-2-^{13}C,^{15}N, >99 atom % ^{13}C, >99 atom % ^{15}N

L-Alanine-2-^{13}C,^{15}N, >99 atom % ^{13}C, >99 atom % ^{15}N

L-4-Hydroxyphenylalanine-2-^{13}C,^{15}N, >99 atom % ^{13}C, >99 atom % ^{15}N

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Course Topics
Experimental Observation of Molecular Motions
• Modern NMR techniques: 3D spectroscopy and molecular dynamics
  • Protein crystallography
  • Multisubunit allosteric proteins

Observation of Internal Motions of Biological Molecules
• Dynamics and conformational transitions in allosteric proteins
  • Principles of NMR and dynamics
  • Protein dynamics and reactions • The energy landscape of proteins

Theoretical Analysis of Internal Motions in Biological Molecules
• Introduction to molecular dynamics • Simulations of protein folding
  • Simulating protein and nucleic acid molecular dynamics
  • New programs in MD simulations • Calculation of free energy and binding constants

Motions in Nucleic Acid
• Nucleic acids structure and dynamics
  • RNA NMR spectroscopy

Analysis of Specific Proteins
• Interactions of antifreeze proteins with ice • Mechanism of action of calcium-signaling proteins
  • tat-Protein structure, dynamics and function
  • Protein-DNA complexes: Heteronuclear strategies of the assignment of larger complexes

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Deadline Dates

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* Fax: 650-493-1348, at any hour. Do not use fax for technical contributions to the Newsletter, for the received fax quality is very inadequate.

* E-mail: shapiro@nmrnewsletter.com

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