THE
NMR
NEWSLETTER

No. 496

January 2000

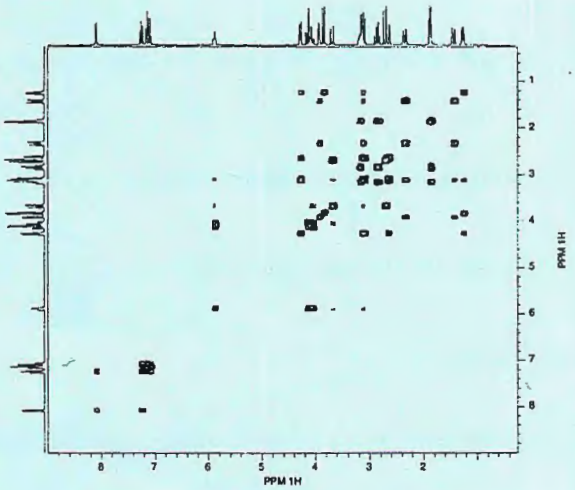
NUTS
Automated Processing

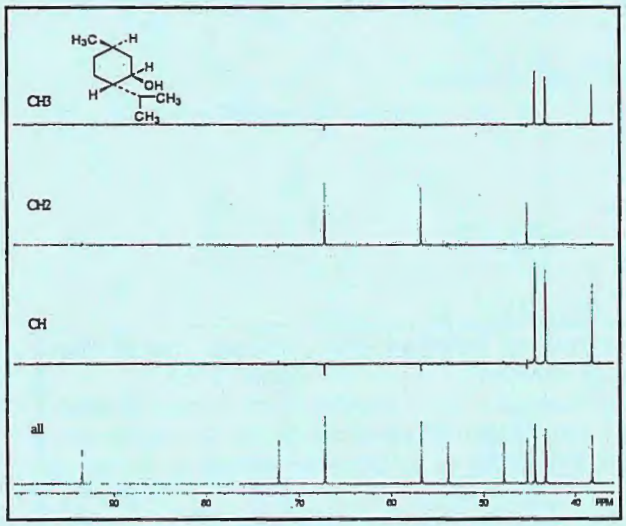
Use macros to

Speed repetitive processing tasks
Customize plots
Process multiple files in batch mode
Calculate composition based on integrals

2D Processing

512 x 512 complex, phase-sensitive COSY processed in ***under 2 sec*** (Pentium II-400)





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FORTHCOMING NMR MEETINGS

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 Center 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.

Symposium on Advances in NMR Applications, Naval Postgraduate School, Monterey, CA. Shuttle service to and from Asilomar will be provided. **April 9, 2000**; Contact: V. Davies, Nalorac Corporation, 837 Arnold Drive, Suite 600, Martinez, CA 94553; 925-229-3501; Fax: 925-229-1651; Email: victoria.davies@nalorac.com; http://www.nalorac.com. See Newsletter 495, 28.

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.

continued on inside back cover

UNIVERSITY OF DELAWARE

Department of Chemistry and Biochemistry
Newark, Delaware 19716-2522

Cecil Dybowski
FAX: (302) 831-6335
Voice: (302) 831-2726
E-mail: dybowski@udel.edu

November 30, 1999 (received 12/06/99)

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

Lead NMR of Aqueous Ionic Solutions

Dear Barry,

Over the years, several investigators have observed the variation of the shift of the ^{207}Pb resonance with concentration in aqueous $Pb(NO_3)_2$ solutions. A similar variation is also seen for other ionic lead materials.

In our labloratory, Natalie Altounian and Alicia Glatfelter have carefully measured shift as a function of both concentration and temperature. At all temperatures and concentrations, there is a single sharp resonance. The shift is interpreted in terms of the equilibrium between the aquated ions and an ion-pair:

$$Pb(NO_3)^+ \longleftrightarrow Pb^{2+} + NO_3^-$$

The problem in doing the analysis was how to determine shifts of each lead species, knowledge of which would allow calculation of equilibrium constants. They got estimates of these by extrapolating to infinite dilution and to high nitrate concentration in solutions with added nitrate. Using these limiting shifts, at each concentration and each temperature, they calculated an apparent equilibrium constant. The temperature dependence of the equilibrium constant at each concentration gave a slightly concentration-dependent apparent enthalpy of reaction. Extrapolation to infinite dilution gives an enthalpy of +0.6 kcal/mole, in agreement with an old electrochemical measurement. A similar interpretation was given for the temperature and concentration variation of the shifts of lead acetate by Harrison's group at the University of Nottingham.[1] It would appear from these results that the lead NMR shift is indicative of the equilibrium between the ions and the ion pair in solution, a process which can be characterized thermodynamically with NMR spectroscopy, even for very small enthalpies.

Yours truly,

Cecil

Cecil Dybowski

---

1 P. G. Harrison, M. A. Healy and A. T. Steel, *J. Chem. Soc., Dalton Trans.* **1983**, 1845.

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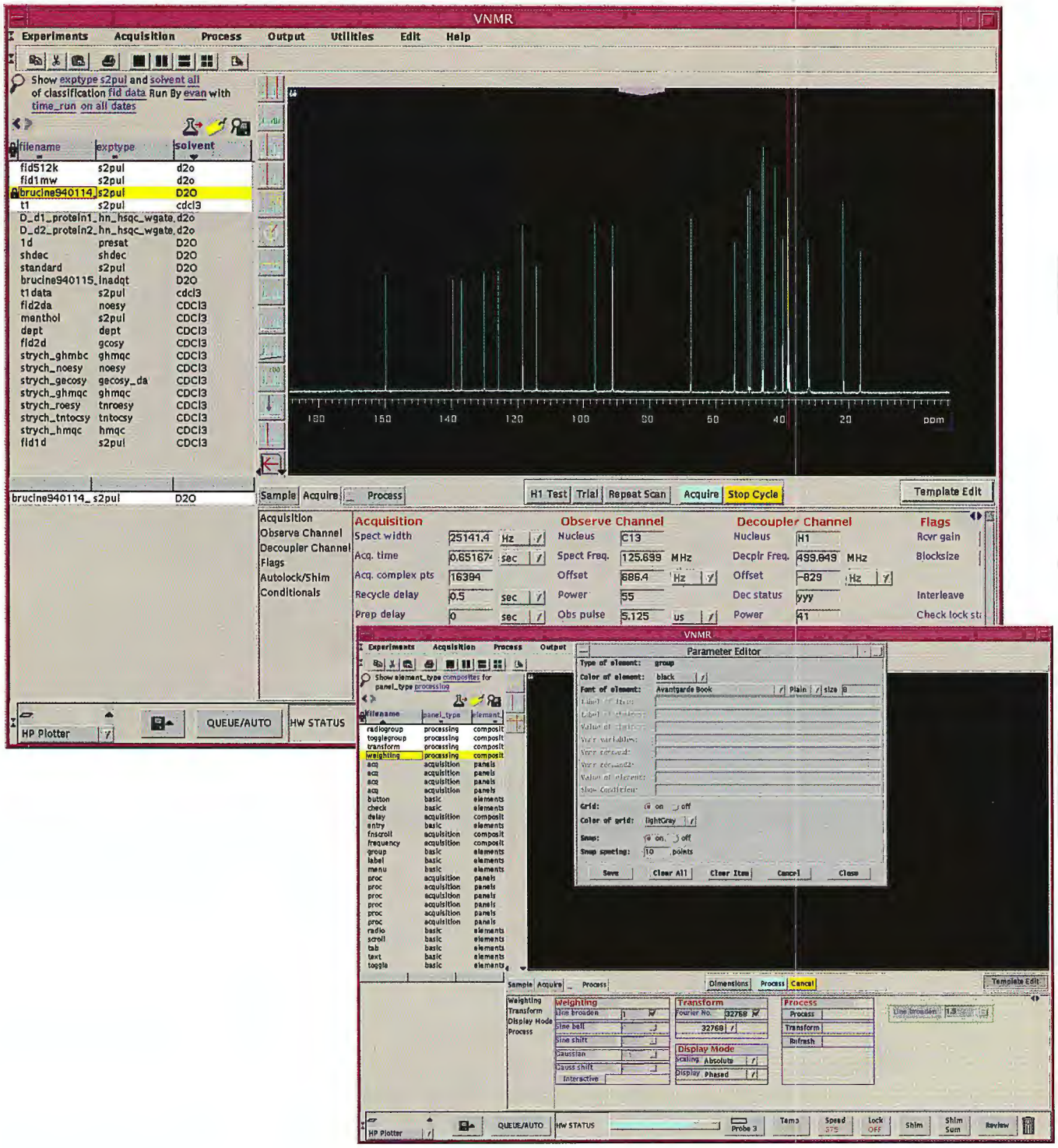

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14 December 1999 (received 12/20/99)

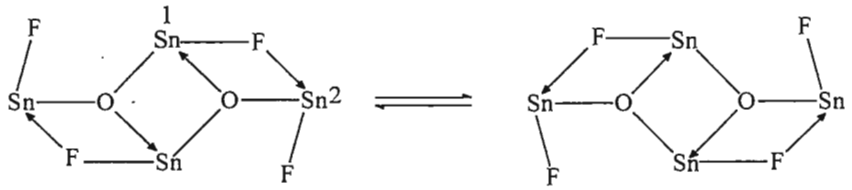
Dr. B.L Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

Re: ^{119}Sn NMR of $\{[^{n}Bu_2SnF]_2O\}_2$: Past and Present

Dear Barry:

I left Dow Chemical a year ago and have relocated to the University of Missouri-Rolla. We recently installed a Varian INOVA 400 spectrometer. I have been busy training students and other faculty members on how to use our new toy as well as attempting to keep our older instruments running.

I am continuing my work on the solution and solid-state structure of dimeric distannoxanes, $\{[^{n}Bu_2SnX]_2O\}_2$ (X = F, Cl, Br), and the composition of their binary mixtures. The 223.66 MHz ^{119}Sn NMR spectrum of 0.125M $[^{n}Bu_2SnF]_2O$ (3:1 by volume $CFCl_3/CDCl_3$) as a function of temperature is shown in Figure 1. The two apparent triplets observed at –146.0 and –162.9 ppm (at 283K) are assigned to Sn1 and Sn2, respectively. The observed splittings, 1800 and 769 Hz, are averaged ^{119}Sn-^{19}F couplings due to the intradimeric distannoxane rearrangement that is extremely rapid at 283K. Reducing the temperature



intradimeric distannoxane rearrangement

causes the linewidths to increase uniformly. This observation indicates that at lower temperatures the broadening is not the result of slowing the intradimeric distannoxane rearrangement, but due to lifetime broadening (short T_2). The ^{19}F NMR spectrum, which is comprised of a narrow singlet ($\Delta\nu_{½}$ = 98 Hz) at room temperature, broadens sufficiently at 173K to disappear into the baseline. The interdimeric exchange of the F ligands is detected by broadening of the multiplets as the concentration of $[^{n}Bu_2SnF]_2O$ increases, see Figure 2. This behavior is mimicked in the concentration dependence of the ^{19}F NMR spectrum as well the ^{119}Sn and ^{19}F NMR spectra at elevated temperatures in ODCB-d4.

At 14.1T the entire ^{119}Sn NMR spectrum is effortlessly obtained allowing straightforward interpretation. However, prior to the advent of high field spectrometers, this was not always the case. The first ^{119}Sn NMR spectra of these important catalytic and biologically active compounds were obtained using a CW spectrometer at 12 MHz in 1963.[1] Only a qualitative description of the ^{119}Sn NMR spectra of $[^{n}Bu_2SnCl]_2O$ and $[^{n}Bu_2SnBr]_2O$ was provided while no comment was made regarding the appearance of the tin spectrum of $[^{n}Bu_2SnF]_2O$. The appearance of "two broad overlapping bands of equal intensity" in the ^{119}Sn NMR spectrum provided spectral evidence for dimer formation. In 1970 the ^{119}Sn NMR spectrum of $[^{n}Bu_2SnF]_2O$ was obtained by heteronuclear double resonance.[2] For those of you who were not practicing NMR prior to the introduction of high field NMR (a relative term; > 200MHz), heteronuclear double resonance was an indirect detection technique in which the X-satellites of the proton spectrum are monitored as the excitation frequency of the X-nucleus is incremented. The resonance condition of the X-

nucleus is found when the X-satellites of the proton spectrum collapse. Using this technique, the 22.37 MHz ^{119}Sn spectrum of a saturated solution of $[^{n}Bu_2SnF]_2O$ in CCl_4 was reported to contain a single broad resonance, –168 ± 14 ppm. By 1971 it was well known that distannoxanes existed at dimers in solution and the single broad resonance was attributed to two overlapping peaks separated by 9 to 14 ppm. Direct detection at low field (ν_o = 29.65 MHz) provided no improvement: very broad singlet at –156 ppm.[3] In the same paper the ^{19}F NMR spectrum of $[^{n}Bu_2SnF]_2O$ in $CDCl_3$ (0.4 - 1.0 M) was also reported to contain a single broad resonance ($\Delta\nu_{1/2}$ = 84 Hz), located at –132.5 ppm exhibiting two pair of resolved $^{117}Sn/^{119}Sn$ satellites (with ^{119}Sn satellite splittings equal to 795 and 1766 Hz). Simulations of the 22.37 MHz ^{119}Sn NMR spectrum at 0.4 and 1.0 M $[^{n}Bu_2SnF]_2O$ reveal that the interdimeric F exchange totally obscure not only the chemical shift differences of Sn1 and Sn2 but also the large tin-fluorine splittings.

This example illustrates how difficult NMR spectroscopy interpretation was before high field magnets and multiple pulse techniques. We are indeed fortune to benefit from the increased sensitivity, resolution, dynamic range and flexible pulse programmers of present day spectrometers at our disposal.

Sincerely yours,

Dennis L. Hasha

Dennis L. Hasha

P.S. Please credit this contribution to the subscription of Dr. Frank Blum

[1] D. L. Alleston, A. G. Davies, M. Hankock and R. F. M. White *J. Chem. Soc.* **1963**, 5469.
[2] A. G. Davies, L. Smith and P. J. Smith *J. Organomet. Chem.* **1971**, *29*, 245.
[3] V. K. Jain, V. B. Mokal and P. Sandor *Magn. Reson. Chem.* **1992**, *441*, 215.

Figure 1

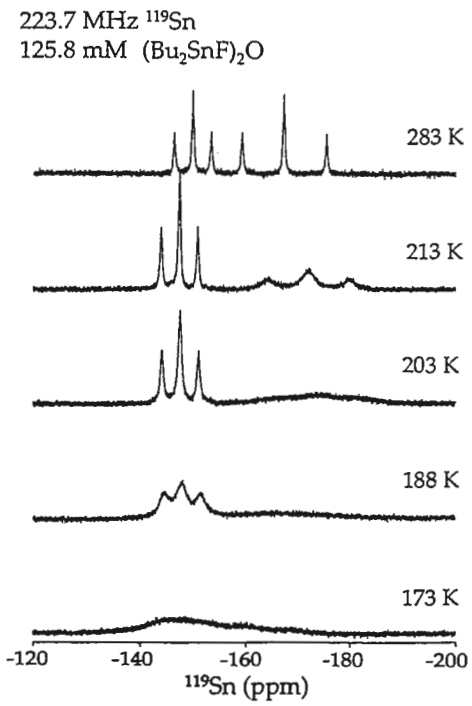
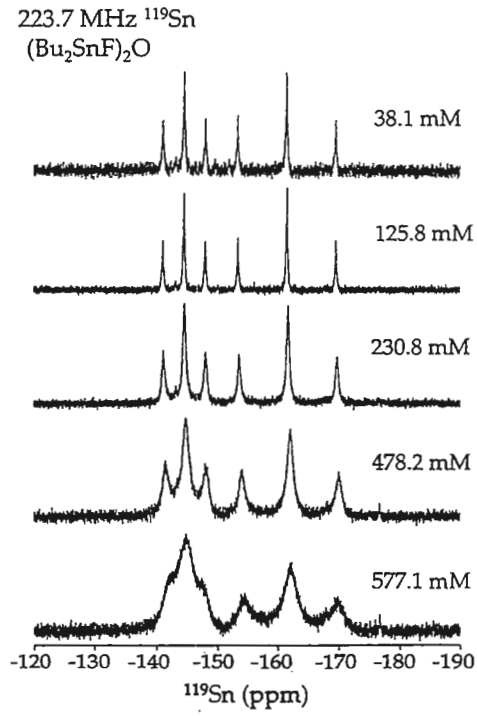


Figure 2



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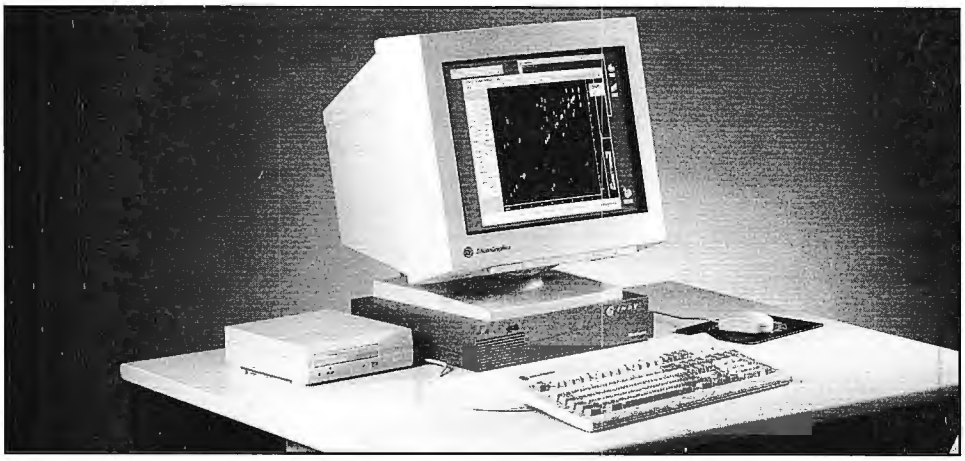

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Dr. B.L. Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

December 22, 1999 (received 12/23/99)

Optimization of a Flow probe

Dear Dr. Shapiro,

During the past year we have moved most of our routine spectral collection from a DRX 500 spectrometer with a conventional magnet and several high resolution probes to a new DRX 600 spectrometer with a shielded magnet, a Gilson sample handler, and a Bruker flow probe. This system has had a dramatic impact on our productivity, both in sample handling/preparation and in the number of spectra collected per day. Sample preparation in a tubeless 96-well plate format is more convenient and reproducible than a series of NMR tubes. In addition, our spectral throughput has increased since the collection time with a flow probe is reduced by three-fourths when compared with the time required to collect the same number of spectra with a high resolution probe and manual sample changing.

The optimization of the flow probe is fairly straight forward, but since some of the readership may not have experience with this probe, we will briefly demonstrate the procedure suggested by Bruker Instruments. Basically, three volumes must be calibrated for each probe as shown in Figure 1. The first is the total probe volume. This is accomplished by injecting a colored liquid into the inlet of a dry probe with a syringe and watching for the liquid to appear in the outlet port (approximately 700-800 μL). This volume is used to calculate the distance required to reposition a sample to the center of the flow cell. The second volume that must be calibrated is the flow cell volume. The stated volume of the flow cell in our probe was 250 μL, but we wanted to determine what volume of liquid was needed to fully fill the coil around the flow cell. To determine this volume, we made repeated injections of a 2 mM sucrose sample and increased the injection volume by 25 μL with each injection. Our flow cell volume was determined to be 300 μL since the peak height of the anomeric proton leveled off around this volume. Once the flow cell volume was determined, we also optimized the positioning volume. The positioning volume can be varied in μL increments to optimize the centering of a sample in the flow cell. This parameter was determined by collecting a series of spectra on a 100 μM sample and varying the positioning volume in 25 μL increments. Samples of these spectra are shown in Figure 2. With our probe, we obtained the best S/N when the positioning volume was set to 25 μL.

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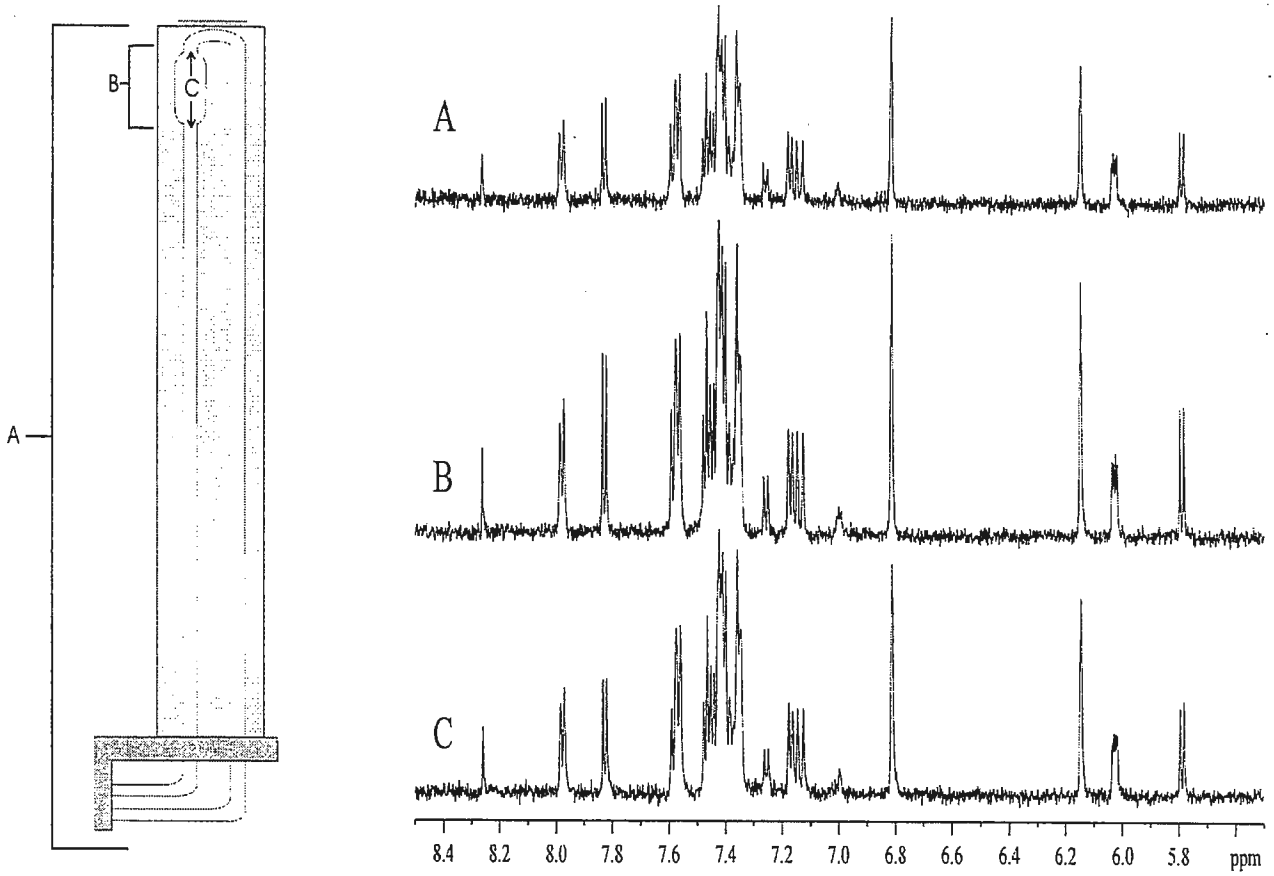

Figure 1. A schematic of a Bruker flow probe showing A) the total probe volume, B) the flow cell volume, and C) the positioning volume.

Figure 2. ^{1}H spectra of a 100 μM sample with the positioning volume set to A) –100 μL, B) 0 μL, and C) +100 μL.

Sincerely,

Kathleen A. Farley
kathleen.a.farley@am.pnu.com

Daneen T. Angwin
daneen.t.angwin@am.pnu.com

Brian J. Stockman
brian.j.stockman@am.pnu.com

P.S. Please credit this submission to the account of Paul Fagerness.

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

November 22, 1999
(received 12/06/99)

Dear Barry,

Overlapped Lines and Resolved Dipolar Couplings – 2D *SLF* in Liquid Crystals

The advantages of working with natural abundance ^{13}C NMR in the case of liquid crystals have been exploited to the hilt by using, among other things, variable angle sample spinning technique for the purpose of determining dipolar couplings and order parameters[1]. For obtaining proton-carbon dipolar couplings from static liquid crystalline samples, we had used an alternative method[2], namely the classical two-dimensional experiment in which the evolution period corresponds to the dipolar oscillations observed during cross-polarisation. This idea has been recently extended further by introducing Lee-Goldburg decoupling during cross-polarisation, which enhances the cross-peak intensities considerably due to reduction in the homonuclear proton dipolar couplings[3]. We have now standardized the method and are able to obtain detailed dipolar coupling information. The method is useful for obtaining dipolar couplings even when lines are overlapped in the chemical shift dimension. An example from our collaborative work with Dr. J-P. Bayle is shown in Figure 1[4], which corresponds to the spectrum at 349 K of the aliphatic part of a liquid crystal designated as ***306***. In the 1-D spectrum peaks due to α and d carbons as well as those due to β and e are overlapped at this temperature. In the 2-D spectrum, distinct cross peaks corresponding to these carbons are clearly observed enabling the corresponding dipolar couplings and order parameters to be measured. We are currently working on methods to obtain local proton-proton dipolar couplings also and hope to communicate to you about this shortly.

Please credit this contribution to the account of Prof.C.L.Khetrapal.

1. *J. Courtieu, J-P. Bayle and B.M. Fung, Prog. NMR. Spectrosc., 26, 141, 1994.*
2. *R. Pratima and K.V. Ramanathan, J. Magn. Resona., A118, 17, 1996.*
3. *C.S. Nagaraja and K.V. Ramanathan, Liquid Crystals, 26, 17, 1999.*
4. *P. Berdague, P. Judeinstein, J-P. Bayle, C.S. Nagaraja, Neeraj Sinha and K.V. Ramanathan, Liquid Crystals (Submitted).*

(K.V. RAMANATHAN) (C.S. NAGARAJA) (NEERAJ SINHA)

email: kvr@sif.iisc.ernet.in

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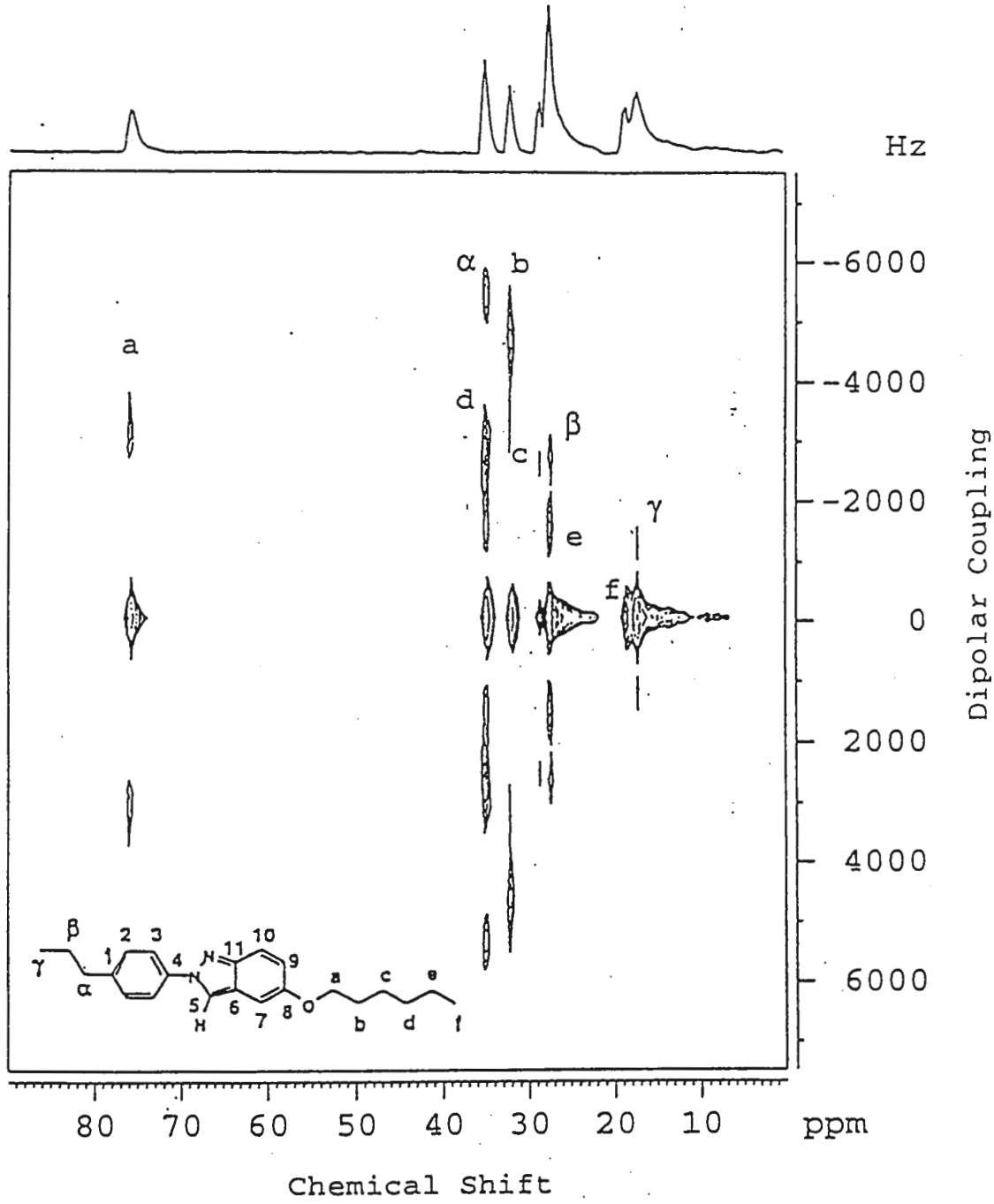
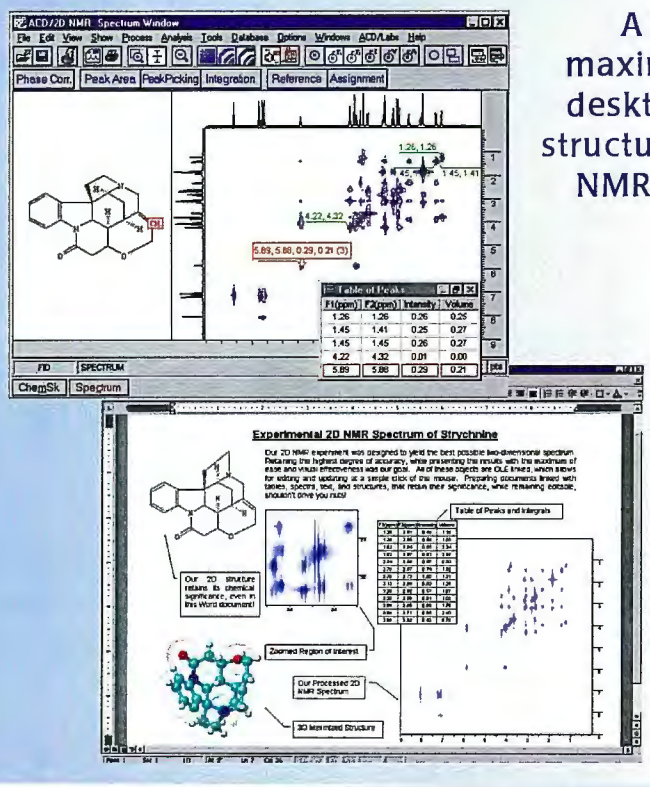


Figure 1: 2D Spectrum of 306 in the nematic phase at 349K.

ACD/2D NMR Processor



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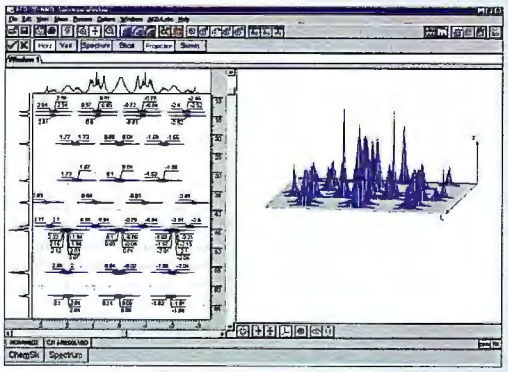

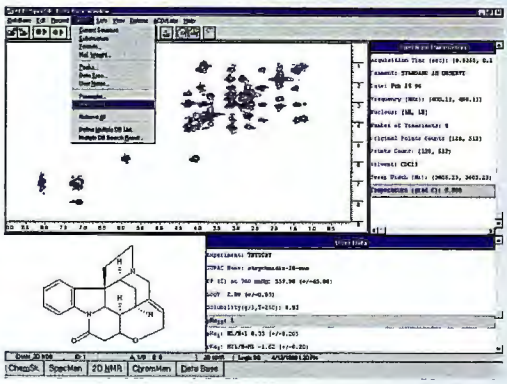

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Email: opella@sas.upenn.edu

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

December 9, 1999
(received 12/10/99)

Improving Isolation in Double-Resonance Probes

Dear Barry,

The isolation between rf channels is one of the most important performance characteristics of a double-resonance probe. Typically, the isolation in double-tuned single coil probes is between 20 dB and 30 dB, and must be supplemented with filters to protect the diodes and preamplifier in high-power solid-state NMR experiments. In this letter, we describe a simple and effective approach to improving the isolation between channels of double-resonance NMR probes.

A conventional double-resonance probe circuit is diagrammed in Figure 1. This circuit utilizes series match and parallel tune for both rf channels, with a shorted quarter wave line to ground on the high frequency side. A trap serves to back-up the low frequency (^{15}N) channel tune capacitor to ensure proper grounding of the high frequency (^{1}H) channel.

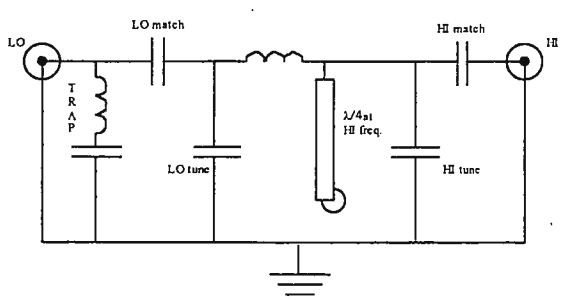

Figure 1: Diagram of a double-resonance circuit.

The isolation between rf channels can be readily optimized by measuring the high frequency isolation as a function of the frequency to which the high side is tuned. This is illustrated in Figure 2. In this example, the initial resonant frequency of the trap is 354 MHz, about 6.5 MHz lower than that of the high frequency rf channel of the probe. Reducing the inductance of the trap brings the resonant frequency close to 360 MHz. The trap inductor can usually be changed in much smaller increments than the capacitor. In this case, the inductance was reduced by shortening the inductor, which consisted of a 0.1" x 0.4" x 0.007" copper strap, by approximately 0.050". This improved the isolation between the channels to 45 dB, significantly better than what could be obtained ignoring the resonant frequency of the trap.

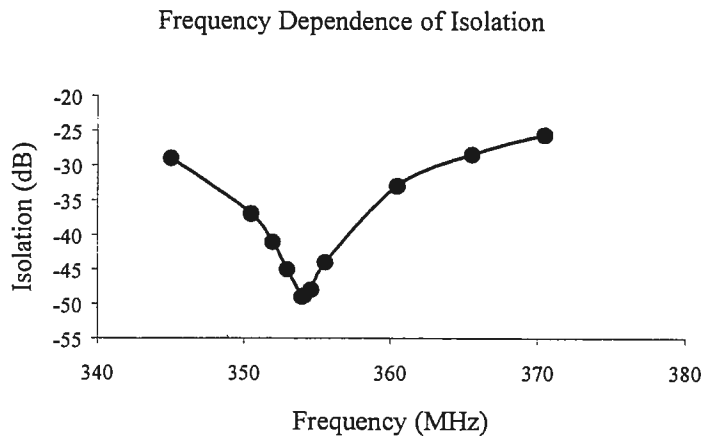

Figure 2: Plot of the isolation between rf channels as a function of frequency before tuning the trap.

The tuning procedure can be summarized as:

1.) Calculate the approximate values of the capacitance and inductance for the trap.

2.) Assemble the probe and tune both rf channels to the desired frequencies using the calculated values for the trap.

3.) Measure the frequency dependence of the isolation between the channels to guide the tuning of the trap.

4.) Tune the resonant frequency of the trap by changing the inductor; if a large frequency correction is needed, then the capacitor may have to be changed as well.

This research is supported by grants P41 RR09793 and RO1 RR12599 from the National Center for Research Resources at the National Institutes of Health. It utilized the Resource for Solid-State NMR of Proteins at the University of Pennsylvania.

Sean T. Burns

Stanley J. Opella

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04103 Leipzig

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

Leipzig, 25.11.99
(received 12/01/99)

Petroleum and Pulsed Field gradients

Dear Barry,

we were recently interested in the applications of pulsed field gradient (PFG) and diffusion-ordered NMR spectroscopic (DOSY) techniques for the analysis of petroleum products including distillate fractions (1), and lubricating oils containing various classes of additives. The techniques have enormous potential (2,3), and can become a supplimentary tool for the analysis of petroleum products, along with the already used routine NMR methods.

Commercial lubricating oil formulations are inevitably a mixture of many components in order to meet various specifications. It is often of interest to determine or at least to varify the presence of various components in such formulations, both in quali- and quantitative terms. The separation of various components becomes a pre-requisite for their further detailed analysis, which is rarely straight forward. Various components encountered in lube oil formulations vary in molecular weights (some time from 200 to 100,000 daltons), and hence PFG NMR offers another possibility for their analysis. The different diffusion coefficients of various additives provide an additional parameter for separating them and simultaneously characterising them.

For example, in a mixture containing triethylene glycol (TEG), di-tertiary butyl phenol (DTBP) and polyoxyethylenesorbitan mono-oleate (POESMO), the resonance signals due to the ethoxylated units of TEG and POESMO are highly overlapped in the region 3-4 ppm. This overlap does not allow the estimation of number of ethoxylated (EO) units present in POESMO, unless it is physically separated from TEG. The separation of such type of components is not straightforward. However, the objective may be achieved using PFG NMR. The conditions of the PFG NMR experiments can be established, wherein, at higher gradient amplitudes, the resonance signals of the faster diffusing components (both TEG & DTBP) can be eliminated from the spectrum, allowing the observation of a clean spectrum of only POESMO. Figure 1 shows the stacked plot comparison illustrating spectral editing for this mixture. In the spectrum using the highest gradient strength, the ratio of the spectral intensity in the region 3-4 ppm with respect to that of 0.85 ppm (terminal methyl of oleate unit) matches exactly with that expected for pure POESMO component.

Sincerely yours

Dr. G. S. Kapur Dr. M. Findeisen S. Berger

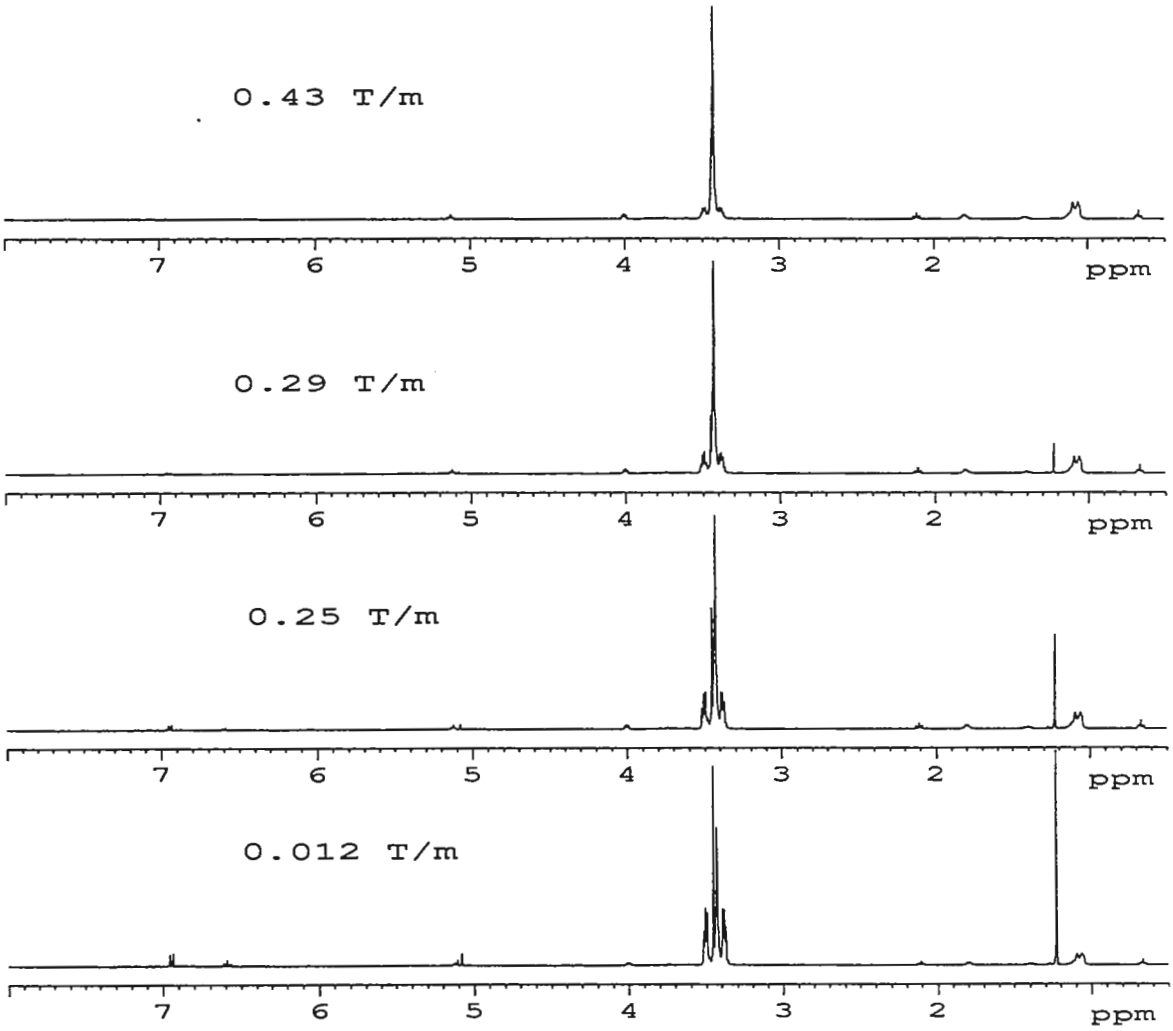

Figure 1: PFG NMR spectra of a mixture of DTBP, TEG & POESMO recorded at different gradient amplitudes.

References

1. G.S. Kapur, M. Findeisen and S. Berger, *Fuel,* 1999 (Accepted).
2. K.F. Morris and C.S. Johnson, *J. Am. Chem. Soc.* 114, 3139-41 (1992).
3. G.A. Morris and H. Barjat, in "Analytical Spectroscopy Library" (Eds. Gy. Batta, K.E. Köver and Cs. Szantay, Jr.), 1997, Elsevier, Chapter 11.

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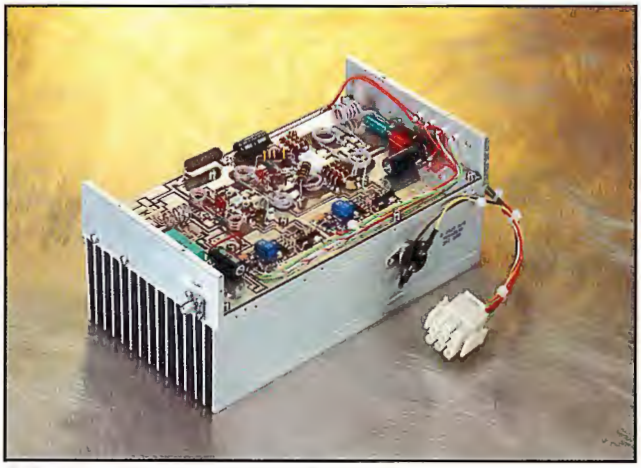

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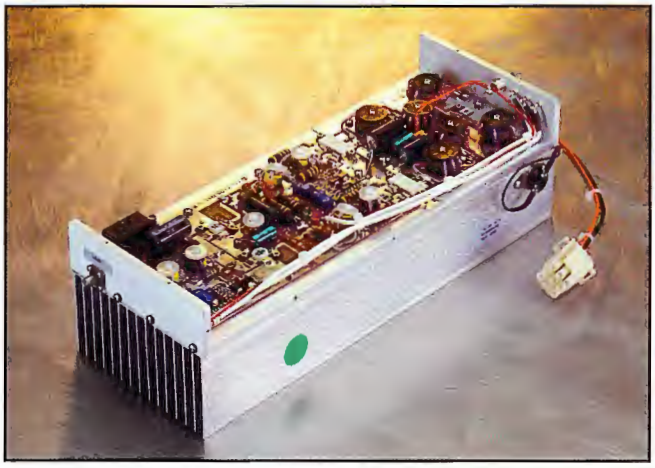

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Professor Bernard L. Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

December 3, 1999
(received 12/08/99)

The benefits of a 180° pre-pulse

Dear Barry:

I would like to sing the praises of what must be one of the oldest tricks in pulsed FTNMR. It is the use of a preparatory inversion pulse alternatingly applied in an add/subtract scheme for suppression of unwanted signals. The sequence is

$$\{- \tau_R - \ldots\ldots - \tau_p - 90° \text{ [Aq+]}$$
$$- \tau_R - 180° - \tau_p - 90° \text{ [Aq−] }\}_n$$

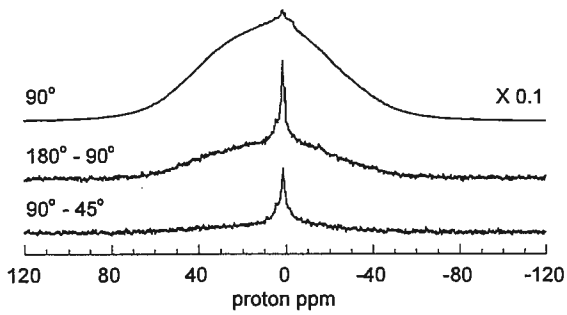
where the dots stand for 'no pulse'. Full signal intensity is obtained if the recycle delay τ_R is much longer than T_1 and the pulse interval τ_p is much shorter than T_1. This simple sequence is known mainly for getting rid of probe ringing, notably with the phase cycling scheme of the RIDE version.[1] I learned about the benefits of the alternating π-prepulse in the mid 1970's when I saw it used in the lab of the late Bob Vaughan at Caltech. For many years it has served us here at DuPont as a very effective means to suppress signals from a variety of unwanted sources. To my surprise I noticed in recent conversations with some of our colleagues that not every NMR spectroscopist is fully aware of its advantages. Hence this brief review in your Newsletter.

For our purposes, the 180° pulse is solely intended to manipulate the z-component of the magnetization just before the observe 90° pulse. Therefore, CYCLOPS phase cycling is applied to the 90° pulse and the detection, while the phase of the 180° pulse is kept unchanged such that any transverse magnetization resulting from the 180° pulse is averaged out.

The accumulated signal intensity of two consecutive FID's is given by $S = 2S_0\exp(-\tau_p/T_1)[1 - \exp(-\tau_R/T_1)]$. This is a bell-shaped curve when plotted against $\log T_1$. Thus when there are signal components with T_1's that differ by an order of magnitude or more, one neatly suppresses the short-T_1 component by choosing an intermediate τ_p. This works well, for instance, for obtaining the deuterium signal of the rigid component in semicrystalline polymers or the ^{27}Al spectrum of the interior of ceramic particles coated with alumina gel. Admittedly, the same result could be obtained by just taking the difference of two spectra with differing recycle delays, but I maintain that this approach offers several advantages including a slight signal/noise improvement, convenience, avoidance of problems arising from long-term spectrometer drift, and overcoming of hardware limitations when the small recycle delay is very short.

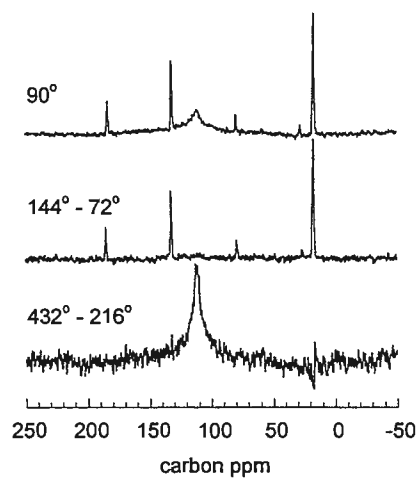
[1] P. S. Belton, I. J. Cox, and R. K. Harris, J. Chem. Soc. Faraday Trans. 2 **1985**, 81, 63.

We use the 180° prepulse not only for T_1 selectivity but also to suppress signals from probe material outside the rf coil. If the rf amplitude is adjusted to produce 180° and 90° pulses in the sample region, then other locations in the probe experience 2θ and θ pulses, where θ is generally smaller than 90°. Material at such locations will give rise to NMR signals with intensity proportional to $\theta \sin^3\theta$, unless T_1 is outside the τ_p-τ_R window, in which case the signal is further reduced. The utility of the background suppression follows from the sharp drop of the function $\theta \sin^3\theta$ when θ decreases below 45°.



As an example, the figure on the left shows 300 MHz proton spectra of a Teflon® plug placed in the sample region of a 7.5 mm rotor in a Chemagnetics triple-resonance probe. It is well known that although Teflon® is nominally proton free, it nevertheless produces a small proton signal, in this case dominated by a sharp peak at 1.3 ppm. The first spectrum is the result of single-90°-pulse excitation. It shows the tiny Teflon® peak on top of a huge broad background signal, presumably from the Vespel® spinning-assembly housing. The second spectrum demonstrates the improvement achieved with the 180°-90° sequence (τ_p = 10 ms, τ_R = 2 s). Cutting both flip angles in half results in an even better background suppression, as is seen in the third spectrum.

Examples of ^{13}C are shown in the figure on the right. They are direct-excitation MAS spectra of a 7.5 mm rotor containing hexamethyl benzene (HMB) and Teflon® (PTFE) endcaps. The 90°-pulse spectrum (top) is cluttered with an unwanted PTFE signal at 112 ppm. Below it is the cleaner-looking spectrum taken with alternating prepulses (144°- 72° flip angles, τ_p = 20 ms, τ_R = 10 s).



The last spectrum demonstrates that our pulse sequence can even be used for some modest depth profiling. Since the rf amplitude generally drops below 50% beyond the edges of a solenoid coil, we can adjust the pulse flip angles so that they are close to180°-90° for the endcaps, while we make the HMB signal ($\theta \sin^3\theta$ integrated over the length of the coil) equal to zero. Taking the rf drop towards the coil ends into account, the latter is achieved when the nominal θ is slightly larger than 180°. In our case it works well for a 432°- 216° pulse pair, as is demonstrated in the bottom trace which shows the PTFE ^{13}C spectrum with near 100% selectivity. Please credit this contribution to the account of Chris Roe.

Best wishes,

Alex

Alexander J. Vega

NATIONAL TAIWAN UNIVERSITY

DEPARTMENT OF CHEMISTRY
1, ROOSEVELT ROAD SECTION 4
TAIPEI, TAIWAN, REPUBLIC OF CHINA
PHONE : 886-2-23635357
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Dr. Bernard L. Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303-3410

December 13, 1999
(received 12/15/99)

Water-filled MCM-41 Characterized by Double Quantum Filtered ^{2}D NMR Spectra Analysis

Dear Dr. Shapiro:

The dynamics of water molecules confined in adsorbed layers of siliceous MCM-41 with a pore diameter of 2.8 nm is investigated at 230 K by deuteron NMR relaxation studies including line shapes of T_1 process and double quantum filtered (DQF) [1] spectral analyses. ^{2}D DQF NMR is a particularly sensitive tool for the determination of the adsorbate dynamics resulting from residual quadrupolar interaction due to the local order. From the study of low loading samples, it clearly demonstrates that analysis of DQF spectra (Fig. 1) provides evidence for the existence of two-compartments in which water is exchangeable. Furthermore, in low loading MCM-41 systems, water predominantly fills the pore surface sites and forms a monolayer. The monolayer water is composed of two different water compartments, i.e. they are characterized by the water, with isotropic reorientational motions, exchanging with the water displaying a solid-like spectrum with 4 kHz edge splitting (Fig. 2). One may expect that the latter water is situated on surface sites in MCM-41. The restricted wobbling motion of the D-O is used to describe its dynamics and is one order slower than the isotropic reorientational motion. The capacity of monolayer water is determined as D_2O/MCM-41 = 0.14 by weight. This agrees well with the result obtained from adsoprtion isotherm study by Takahara et al.[2]. For high loading samples, water continuously builds up around the monolayer. For fully filled sample, a considerable number of the water molecules is believed to be at the middle region of the cylindrical pore. The evidence of SQ and DQF NMR analyses reveals the process of water filling and supports the view of smooth wall model for MCM-41[3]. The feature of DQF spectral analysis in conjunction with the usual relaxation studies may be a distinguishing combination of NMR methods for characterizing the dynamics and adsorption interaction in the porous system. This study forms part of a continuing series of NMR studies for the investigation of diffusion and adsorption in porous material.

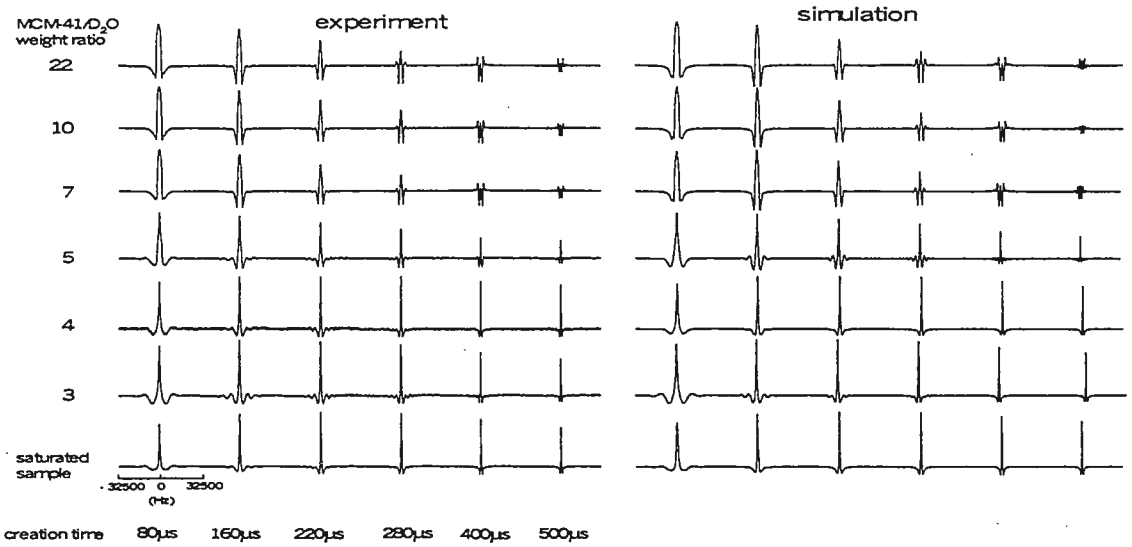

Fig. 1. Experimental (left) and simulated (right) ^{2}D double quantum filtered spectra at various creation time cited for water-laden MCM-41 samples at 230 K. The creation times are cited underneath the spectra. The spectra were acquired at 76.78 MHz

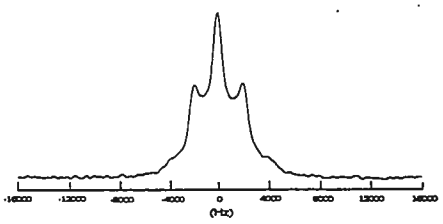

Fig. 2. Typical SQ spectra at 230 K at 46.07 MHz for Water-filled MCM-41 sample (MCM-41/D_2O weight ratio = 10)

References:

[1] Chen, Y. H.; Hwang, L. P. *J. Phys. Chem. B* **1999**, *103*, 5070.

[2] Takahara, S.; Nakano, M.; Kittaka, S.; Kuroda, Y.; Mori, T.; Hamano, H.; Yamaguchi, T. *J. Phys. Chem. B* **1999**, *103*, 5814.

[3] Edler K. J.; Reynolds P. A.; White J. W. *J. Phys. Chem. B* **1998**, *102*, 3676.

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Tsyr-Yan Yu Chi-Yuan Cheng Dennis W. Hwang Lian-Pin Hwang*

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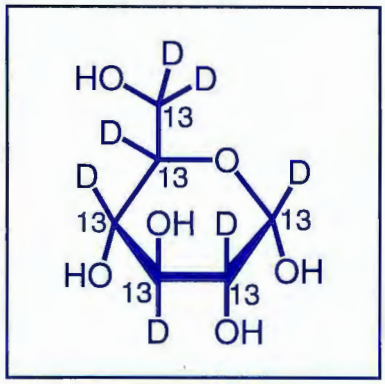

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The University of Sydney
NSW 2006 Australia

Telephone: +61 2 692 2597
Facsimile: +61 2 692 4726

Dr Bernard L. Shapiro
The NMR News Letter
966 Elsinore Court
Palo Alto, CA 94303

(received 12/30/99)

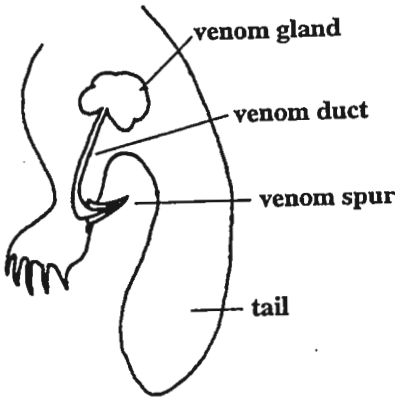
NMR structure determination of defensin-like peptides in platypus venom

Dear Barry,

The Australian duck-bill platypus is a unique mammal that has many reptilian characteristics. Among these features are the laying of eggs, low body temperature of ~32°C, and the presence of venomous spurs on the male hind legs. However, unlike the snake venoms, the platypus venom is only produced during the mating season and is used to assert dominancy over other males. It is also known that the platypus uses these toxic spurs to ward off potential enemies including dogs and humans. The venom is not fatal to humans but is described to cause excruciating pain followed by swelling and hyperalgesia.

We are currently investigating the nature of the platypus venom in order to identify the different components and to shed light on the evolutionary origin of this strange mammal. Although a C-type natriuretic peptide and a nerve growth factor protein have been identified in the venom, many of the proteins and peptides we have found are novel in that they are not similar to those present in other reptilian venoms or to any other proteins. This result clearly suggests that the platypus venom has evolved substantially from its reptilian ancestral venom and also underscores the uniqueness of the platypus in the animal world.

Among the novel peptides identified were a family of four polypeptides of 5 kDa which are present in significant amounts in the venom. We refer to these peptides as defensin-like peptides or DLPs since NMR studies of two member peptides, DLP-1 (1) and DLP-2, revealed that their three-dimensional folds have significant similarities to β-defensin 12, an anti-microbial peptide from bovine neutrophils. DLPs possess no anti-microbial properties and their roles in the platypus venom remain to be established.



Platypus venom apparatus

DLP-1 structure

References

1. Torres, A.M., Wang, X., Fletcher, J.I., Alewood, D., Alewood, P.F., Smith, R., Simpson, R.J., Nicholson, G.M., Sutherland, S.K., Gallagher, C.H., King, G.F., & Kuchel, P.W. *Biochem. J.*, **341**, 785 (1999).

Yours Sincerely,

Allan Torres

Philip Kuchel

Address all Newsletter correspondence to:

Dr. B. L. Shapiro
The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303.
650-493-5971* - *Please call only between 8:00 am and 10:00 pm, Pacific Coast time.*

Deadline Dates

No. 497 (Feb.)	21 Jan. 2000
No. 498 (Mar.)	25 Feb. 2000
No. 499 (Apr.)	24 Mar. 2000
No. 500 (May)	28 Apr. 2000
No. 501 (June)	24 May 2000

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Forthcoming NMR Meetings, continued from page 1:

Gordon Research Conference on Magnetic Resonance, **June 17-22, 2001**, Roger Williams University, Bristol, Rhode Island (note the new, improved location !!!). Contacts: Rob Tycko, Chair, 301-402-8272, tycko@helix.nih.gov, and Kurt Zilm, Vice-Chair, kurt.zilm@yale.edu. Site description and application information available at http://www.grc.uri.edu.

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.

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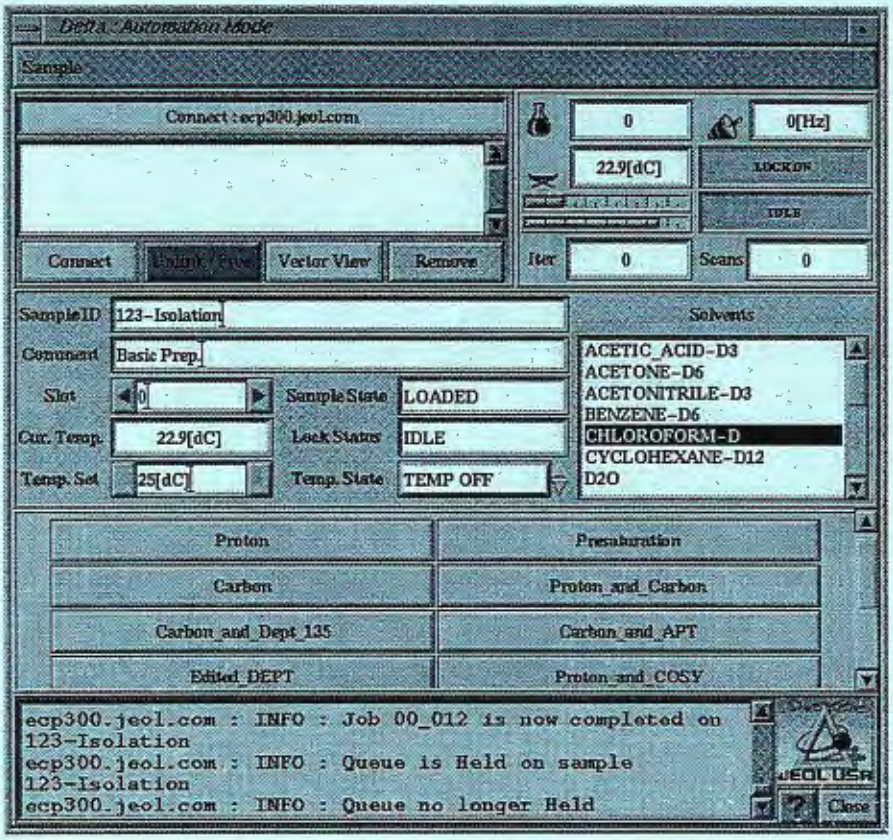

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