THE
NMR
NEWSLETTER

No. 507

December 2000

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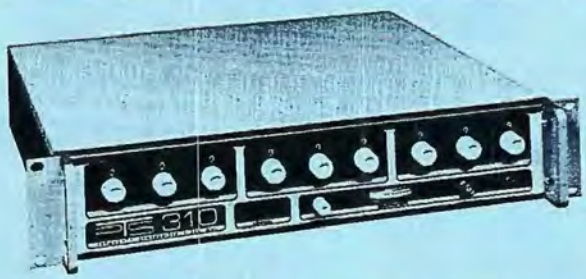

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FORTHCOMING NMR MEETINGS

Frontiers of NMR in Molecular Biology VII, Big Sky, Montana, **January 20-26, 2001**. Contact: Keystone Symposia, Drawer 1630, 221 Summit Place, Suite 272, Silverthorne, CO 80498. Tel: 800-253-0685 or 970-262-1230; Fax: 970-262-1525; E-mail: keystone@symposia.com. http://www.symposia.com.

PITTCON 2001, New Orleans, LA, **March 4-9, 2001.** Contact: The Pittsburgh Conference, Dept. CFP, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235-5503. Tel: 412-825-3220; Fax: 412-825-3224; E-mail: pittconinfo@pittcon.org.

42nd ENC (Experimental NMR Conference), Rosen Plaza Hotel, Orlando, Florida, **March 11-16, 2001**; Arthur G. Palmer, Chair: Agp6@columbia.edu; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87505; (505) 989-4573; Fax: (505) 989-1073; E-mail: enc@enc-conference.org; Web: www.enc-conference.org.

ACS National Meeting, "Symposium on High Resolution NMR Spectroscopy of Polymers, " San Diego, CA, **April 1-5, 2001**; Contact: H. N. Cheng (hcheng@herc.com) or A. D. English (alan.d.English@usa.dupont.com); See Newsletter 505, 29.

Magnetic Resonance in Chemistry and Biology, XIth International Conference, Zvenigorod, Russia, **April 20-27,2001.** Contact: http://www.nmr.de/html/conf/zelino.shtml.

ISMRM 9th Scientific Meeting and Exhibition; ESMRMB 18th Annual Meeting and Exhibition, Joint Annual Meeting. Glasgow, Scotland, **April 21-27, 2001**.Contact: ISMRM Central Office, 2118 Melvia Street, Suite 201, Berkeley, CA 94704. Tel: 510-841-1899; Fax: 510-841-2340; E-mail: info@ismrm.org.

Computational Aspects of Biomolecular NMR, Gordon Conference, "Il Ciocco", Barga (Pisa) Italy, **May 6-11, 2001.** Contact: Michael Nilges nilges@embl-heidelberg.de, or Dave Cast case@scripps.edu.

ISMRM 9th Scientific Meeting and Exhibition, and ESMRMB 18th Annual Meeting and Exhibition, Joint Annual Meeting, **April 21-27, 2001**, 10th Annual Meeting of the Section for Magnetic Resonance Technologists, and 17th Annual Meeting of the British Association of MR Radiographers, **April 20-22, 2001** Glasgow, Scotland, UK; Contact: ISMRM, P.O. Box 45690, San Francisco, CA 94145-0690; http://www.ismrm.org

continued on page 28

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Zürich, 10.11.2000

(received 11/21/2000)
2515

Dr. B.L. Shapiro
The NMR Newsletter
966 Elsinore Court

Palo Alto, CA 94303-3410
U.S.A.

MatNMR: a flexible processing package for MATLAB

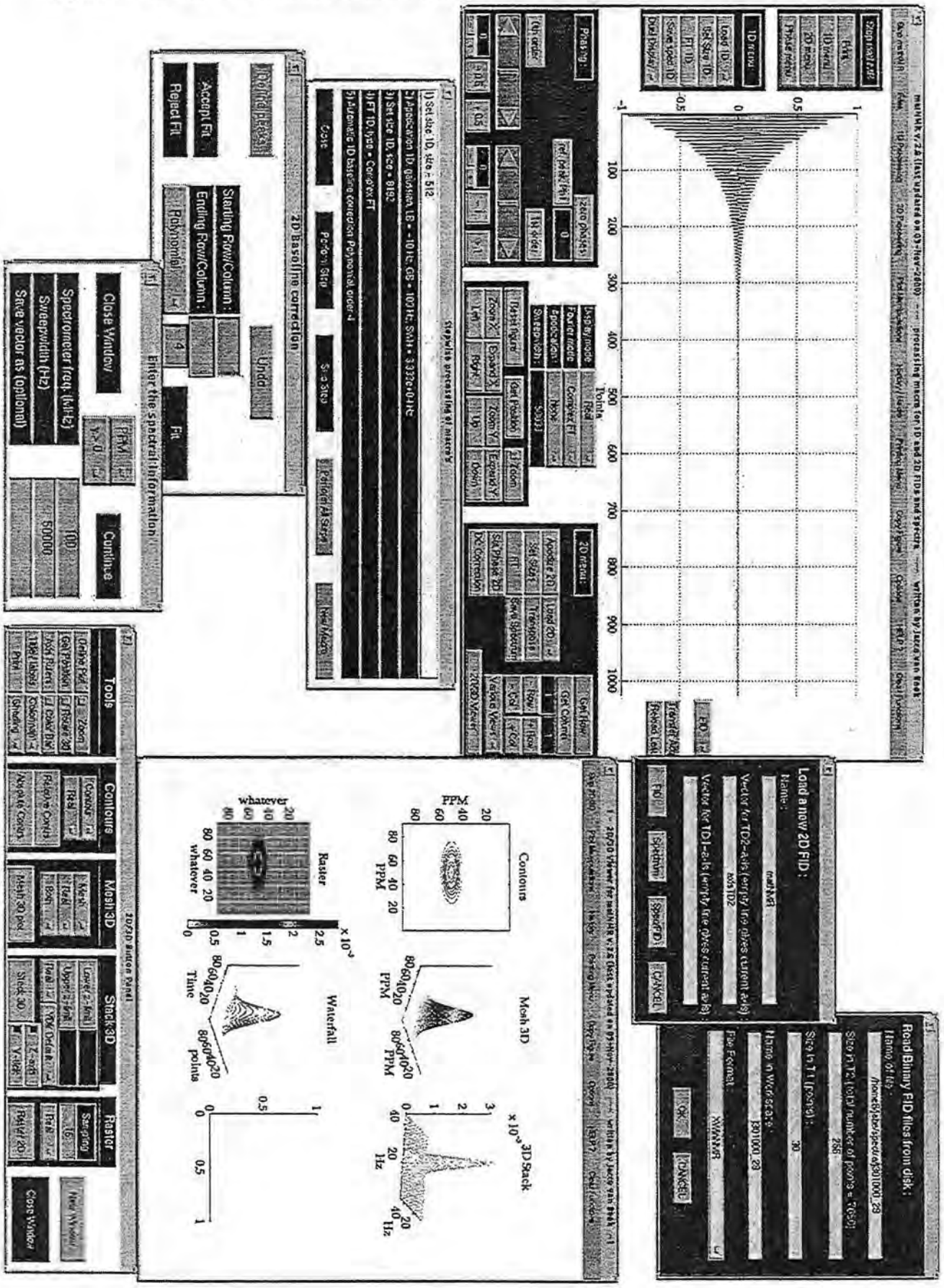
Dear Dr. Shapiro,

We often use MATLAB to process our NMR data. This software package is well suited for numerical computation and visualization. In particular it is optimized for doing matrix calculations of all sorts. In this contribution we would like to bring to the reader's attention a package that we have developed for processing and visualizing 1D and 2D NMR/EPR data in MATLAB.

MatNMR is a flexible processing toolbox with a graphical user interface. Most of the functions used for processing by commercial packages have been implemented (input filters for various spectrometer file formats, various Fourier transforms, baseline corrections, shearing transformation, linear prediction, peak fitting, T1-fitting, etc.) and user-defined functions can easily be added. Although in principle processing is done step-by-step, macros can be defined for automated processing. Furthermore matNMR keeps track of the processing history for each spectrum. Saving this with the FID avoids having to write all details in a lab journal and makes saving of the spectrum (which is usually much bigger in size than the FID) unnecessary as it can be reprocessed fast at a later time when loading the FID into MATLAB.

Its flexibility originates from what is called the "workspace" in MATLAB: a virtual space where any variable (number, vector, matrix etc.) that is created by the user is stored with its own name, and can be manipulated at any time. As matNMR operates in the same workspace any

Fig. 1: a selection of screenshots from matNMR



variable that matNMR uses, e.g. the spectrum, can at any time be changed manually, if wanted. This also invites for user-defined functions to be used in combination with matNMR. All in all this gives the user complete control over the data. Although using this flexibility to its maximum requires (some) knowledge of MATLAB, it is not really a prerequisite for working with matNMR. Indeed, in our experience most people quickly learn and like how to work with matNMR.

For visualization matNMR offers an unlimited number of multi-plot windows with routines for making various types of contour plots and 3D plots. MATLAB offers a far greater span of graphical functions though and they can be used in combination with matNMR by giving the appropriate syntax from the MATLAB prompt. The appearance of the figures can easily be changed either by using the functions supplied by matNMR or again by using the corresponding MATLAB commands directly.

Relatively small sized spectra are the principal scope of matNMR. All processing is done in the memory of the computer and not on disk as most other programs do. Processing spectra of for example 2k*2k points, can easily amount to 256Mb of memory usage or more under UNIX (under MS Windows it seems to be more efficient though). This may require some care therefore. The source code is platform independent. It runs on all platforms which are supported by MATLAB, e.g. UNIX, Windows 95/NT, Mac. Furthermore it is small (version 2.6 is approximately 1.4Mb (uncompressed)) and no additional compilers or installation steps are necessary except copying it to a disk and setting the MATLAB path to it. MatNMR is free of charge and is distributed under the GNU public license.

More details, including a manual, are given on the web site at http://www.nmr.ethz.ch/matnmr. From there also the source code can be downloaded directly. The current version is 2.6 and requires MATLAB 5.2 or higher (older versions are still available). For more questions and remarks regarding matNMR please contact Jacco van Beek, jabe@nmr.phys.chem.ethz.ch.

Sincerely,

J v. Beek

Jacco van Beek

Beat

Beat Meier

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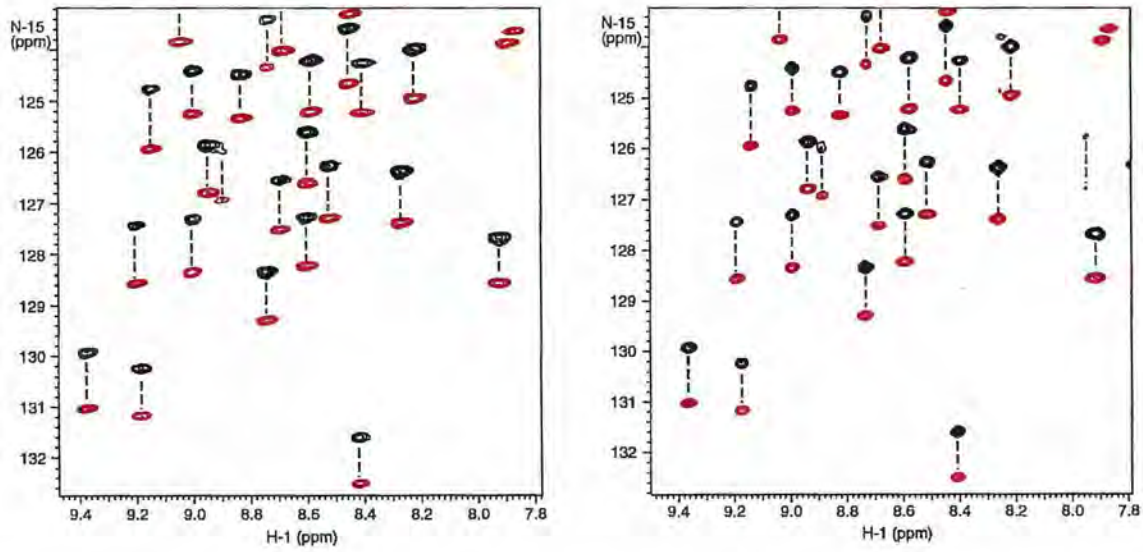
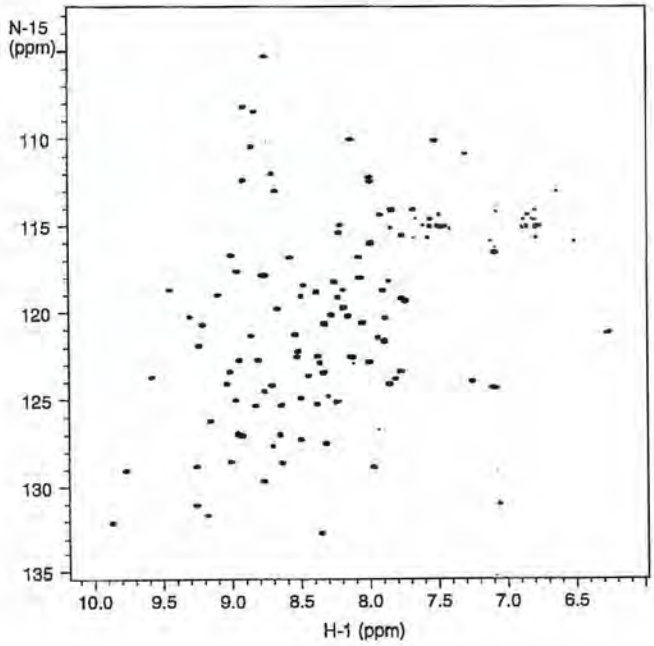


Measurement of residual dipolar N-H couplings at 900 MHz in partially oriented proteins with (right) and without the use of band-selective homonuclear decoupling.

TROSY at 900 MHz



The ^{15}N-^{1}H TROSY correlation spectrum of 6F1 1F2 module pair from the gelatin-binding domain of fibronectin. Sample courtesy of Prof. .I.D. Campbell of Oxford University.

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November 30th, 2000
(received 11/30/2000)

Automated First-Order Multiplet Analysis

Dear Barry,

We are all well aware that the dependence of the values of NMR spin-spin coupling constants on molecular conformation can be a valuable tool in the structure determination process. The continuing increase in the resonance frequency of modern NMR spectrometers allows more and more resonances to be examined using first-order multiplet analysis. While this can easily be done for the simplest patterns (doublets, triplets, quartets), more complex patterns can be extremely difficult to analyze. This is certainly an issue for synthetic organic chemists accessing walk-up spectrometers and who have not received the appropriate training in spectral analysis.

The task of deducing the coupling constant values from a multiplet is the reverse process of generating a conventional splitting tree from a single line (chemical shift) by sequential branching using a given set of coupling constants. While the latter process is dealt with in numerous textbooks, see for example [i], the more complex task of constructing the inverted splitting tree has received much less attention. Although the general protocol of inverted splitting tree generation was published several years ago [ii], it does not seem to have found widespread use.

Outlined here is a simple straightforward method of deducing coupling constant values from first-order multiplets. It is based on the general inverted splitting tree algorithm [2], but includes also a peak intensity normalization procedure. For the success of the inverted splitting tree algorithm it is crucial to have as an input a list of correctly normalized peak intensities such as 1:3:3:1 in the quartet case. The peak normalization of more complex coupling patterns presents significant difficulties.. The main reasons for this are the distortion of the peak intensities and the necessity to know the number of couplings giving rise to a multiplet under analysis. It is helpful to use the number of peaks in a multiplet to determine the smallest possible number of couplings. According to the first-order rules [1] N coupling constants would give no more than 2^N peaks, so when there are 9 peaks in a multiplet one would expect at least 4 coupling constants involved. Intensity distortions are probably the most complex issue to resolve. It is rare that the peak heights (or even the peak areas after spectrum deconvolution) give relative ratios close to integer numbers. To account for this we have developed a procedure that utilizes multiplet symmetry and generates a set of possible first-order intensity distribution patterns. When combined together with a inverted splitting tree algorithm it is possible to find an intensity pattern that allows deduction of a proper set of coupling constants.

Initial testing of this approach has proved the algorithms to be very robust. We have been able to automatically determine up to seven different values of the coupling constants allowing us to decipher even the most complex coupling patterns. One challenging complex multiplet is shown in Figure 1. This spectrum was obtained after accurate phasing and baseline correction, which of course are the prerequisite for any quantitative analysis.

Although the experimental multiplet appears symmetrical one can observe a number of significant wiggle-type distortions. However, the procedure was still able to find a solution. Indicated at the top of the Figure 1 is a multiplet calculated with experimentally determined coupling constants. J = 5.37 Hz originates from the methyl group while J = 6.74 Hz is due to the

two methylene groups. The two spectra strongly resemble each other confirming the reliability of the solution.

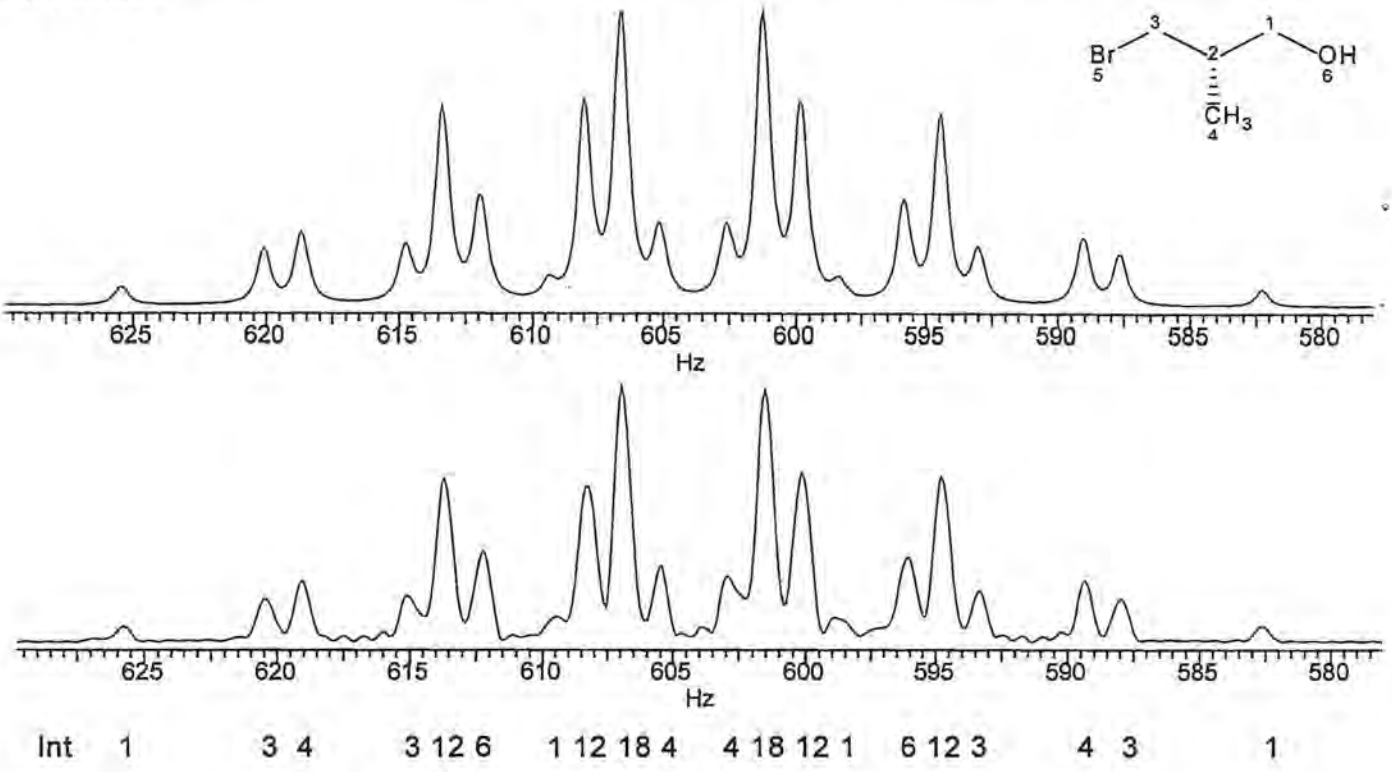

Figure 1. The experimental 1H NMR 300 MHz subspectrum of the methine proton of 3-bromo-2-methylpropan-1-ol. The multiplet is simulated with the parameters $\delta = 2.01$ ppm, J1 = J2 = J3 = 5.37, J4 = J5 = J6 = J7 = 6.74 Hz (top). Given below the experimental spectrum are the relative intensities of the peaks calculated by the normalization procedure.

Automated multiplet analysis of this type will be of great value for the interpretation of spectra, especially in the hands of non-specialists who are struggling to interpret a complex pattern. We have previously delivered H1 NMR prediction capability and the ability to compare directly onscreen experimental and predicted spectra. We believe that the analysis tool developed here will offer an additional level of visualization and analysis to aid in the facile analysis of NMR spectra. We hope to make this capability available in our next release of software.

Yours sincerely,

Antony Williams, Eugene Vodopianov, Sergey Golotvin
Advanced Chemistry Development

References:

i E.D. Becker, High Resolution NMR, Acad. Press, 2000.
ii T.R. Hoye, P.R Hanson, and J.R. Vyvyan, J.Org.Chem, 1994, 4096

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Department of Physics

(received 11/18/2000)

10th November 2000

Powder Alignment In The Field

Dear Barry,

We saw the darnedest thing while studying a metal-deuteride, $ZrBe_2D_x$, with a hexagonal layered crystal structure. Because of the metallic electrical conductivity, the sample is used as a powder, for good rf B_1 field penetration. When we examined the ^9Be (spin 3/2) resonance in an 8.0T field, we found that our relatively weak rf field ($\gamma B_1/2\pi$ = 25 kHz, as determined on a solution of $BeSO_4$ in water) was hitting primarily (but not exclusively) the central transition. But as you can see from Fig. 1, the satellite resonances (m = ±1/2 to ±3/2 transitions, 144.5 kHz above and below the central) appear as high frequency beats on top of the central transition's FID. The pulse was kept short (3 μs), to improve the excitation of the satellites. These satellite FID's are surprisingly long, much longer than expected for a Pake powder pattern. Could it be that the crystallite grains are being aligned by the static field B_o ?

To test this, we prepared a sample in which the particles were prevented from reorienting by being tightly packed (after first being randomly oriented by shaking). The long satellite FID's are not present in the sample (data not shown). So the loosely packed sample really is aligning in the field.

We also made a sample loosely filled with powder and immersed in C-18 alkane (m.p. 30 °C). At 50 °C the alkane is liquid and the particles align in the field as before. The temperature is reduced to nearly 0 °C, the alkane freezes, and the alignment is locked in. We prefer this over epoxy glues, since there is a limited quantity of sample and epoxies don't come off easily. In Figs. 1 and 2 the FID is presented for the frozen-in sample at 0 and 30 degrees from the initial alignment. The broadening of the satellite FID

FIG 1

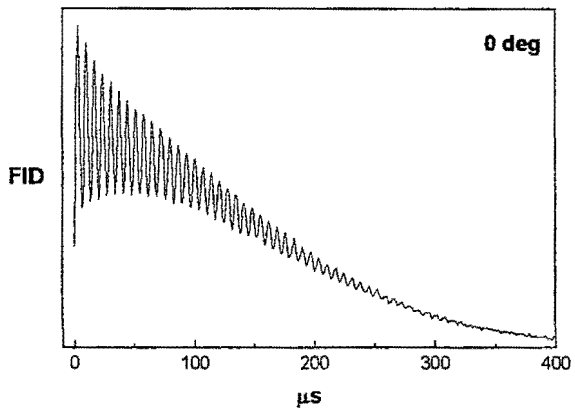
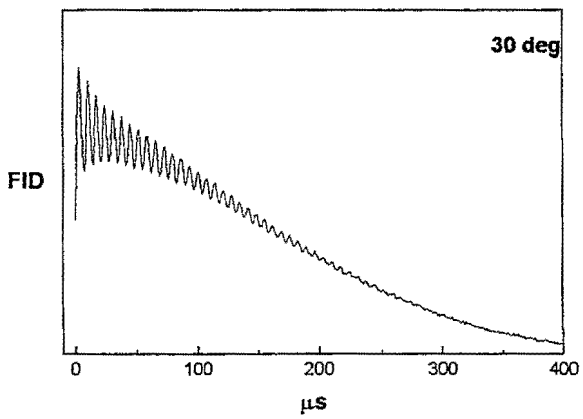


FIG 2



at 30° is evident from the decreased amplitude of the satellite beat.

The unique axis of the electric field gradient (EFG) tensor is no doubt parallel to the crystalline (hexagonal) c-axis, from site symmetry considerations. The rotation data, such as Figs.1 and 2, prove that the c-axes align perpendicular to B_o. If the c-axes were parallel to B_o, all the EFG unique axes would have a unique orientation; the satellite frequency would vary as $(3\cos^2\theta - 1)/2$, for sample tube reorientation by angle θ about an axis perpendicular to B_o, as in our NMR probe. This prediction disagrees with the data of Figs. 1 and 2 (the long-time beat frequency is unchanged at $\theta = 30°$). On the other hand with c-axes perpendicular to B_o, one expects the c-axes to be more or less randomly distributed in the plane perpendicular to B_o. Thus, rotation to $\theta = 30°$ (e.g., as in Fig.2) will result in a distribution of angles (from c-axes to B_o) from 60° to 120°. The c-axes near 90° (a turning point) will continue to create a sharp cusp in the frequency spectrum and a slowly decaying FID component at 144.5 kHz, in agreement with Figs. 1 and 2. The lack of a second cusp frequency corresponding to 60° and 120° demonstrates incomplete particle alignment by the field.

The sample of Figs.1 and 2 was initially immersed in molten C-18 alkane with the sample tube held vertical outside the magnet. We believe the flake shaped particles tend to be oriented initially horizontally (c-axes along gravity). The solidified sample was then put into the NMR probe, inserted into the field, melted and allowed to field align, and then frozen to 0°C. Thus, with the sample in the NMR probe (tube axis now horizontal), there will be a preponderance of c-axes parallel to the tube axis (and still perpendicular to B_o). This effect reduces the decrease in beat amplitude for angles away from zero.

FIG 3

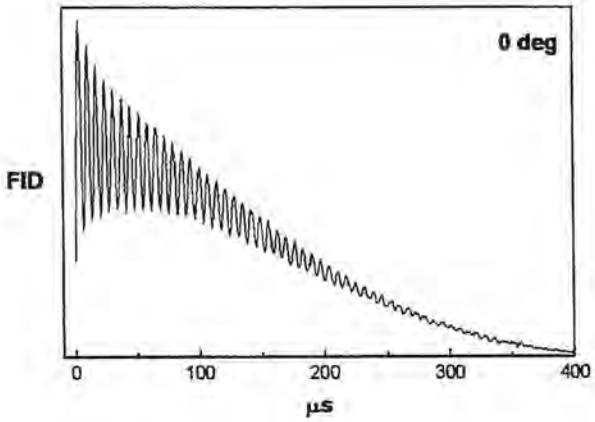
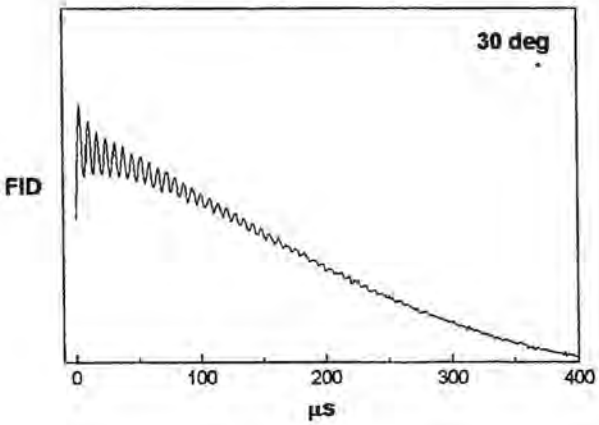


FIG 4



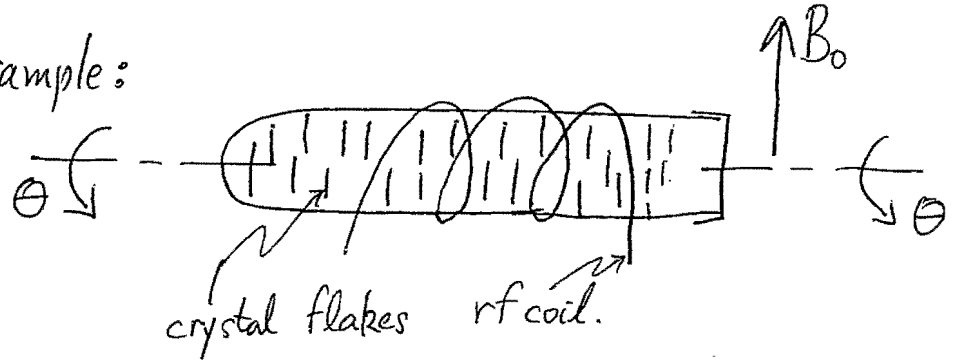
Indeed, we prepared the same sample a second way, by allowing the alkane to freeze with the tube-axis horizontal, outside the field. This sample, after field alignment, shows a larger variation with sample-tube rotation (Figs. 3 and 4). We believe this sample has c-axes after field alignment more nearly at all angles in the plane perpendicular to B_o.

What surprises us here is (i) the extent of alignment of the sample as evidenced by the sharp satellites and (ii) that such a nominally non-magnetic system should align at all (Zr? Be? D?). We note that field alignment in epoxy is widely used with the high-Tc superconductors, but there, magnetic effects are definitely expected.

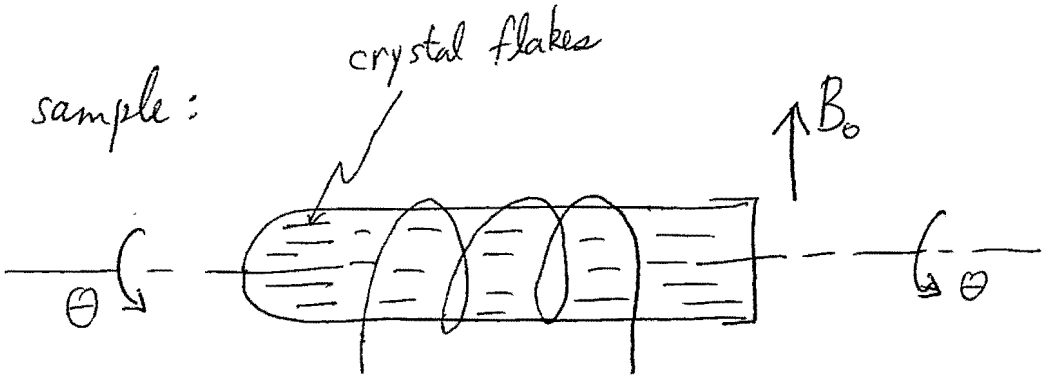
Sincerely,
Vikram Kodibagkar and Mark Conradi

Sketch of initial alignment of flat flakes, before field-alignment.

1st sample:



2nd sample:



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To be held prior to ENC at the
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Sunday, March 11, 2001
1:00 to 6:00 p.m.

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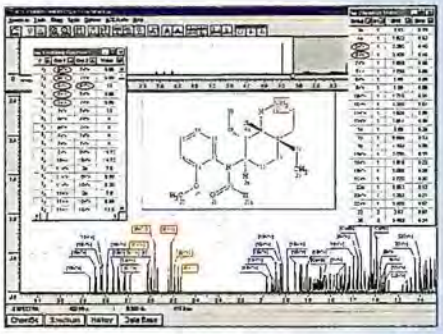
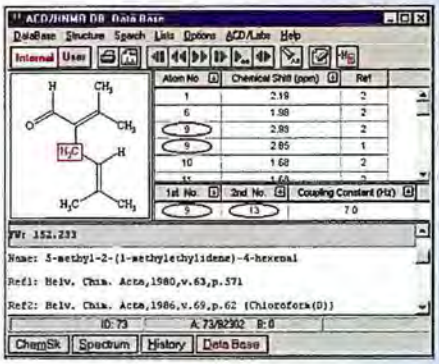


View coupling constants with highlighted atoms



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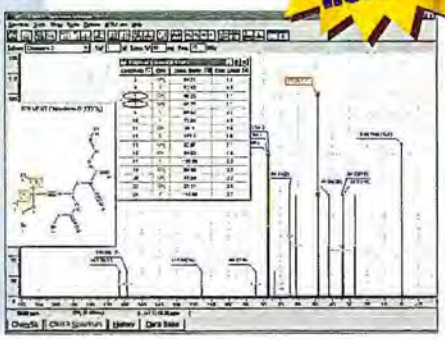
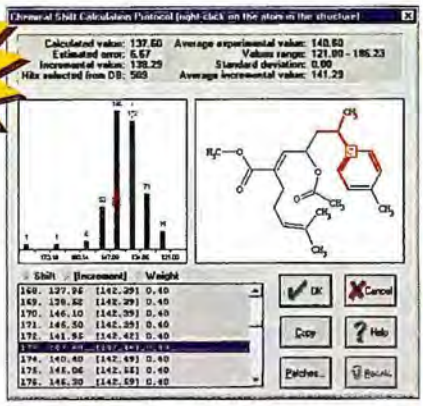
- **ALSO AVAILABLE!** The proton and carbon NMR DB Add-ons now contain the user-accessible ACD databases of over 100,000 structures (**NEW**- an increase in size of 20% for HNMR, and an increase of 50% for CNMR, compared to version 4.0). These DBs include original references, molecular formula, molecular weight, IUPAC name, coupling constants (if applicable), NMR experiment (technique, frequency, temperature) and trivial name, all of which can be viewed and printed out.
- For CNMR, the ACD/Natural Products DB Add-on contains over 5,200 structures from marine and terrestrial sources.

Version 4.5 Release!



Verify shifts & coupling constants with on-screen structural relation



Protocol Window explains the calculation procedure

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NMR

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Look up structures and predict spectra from the same interface!

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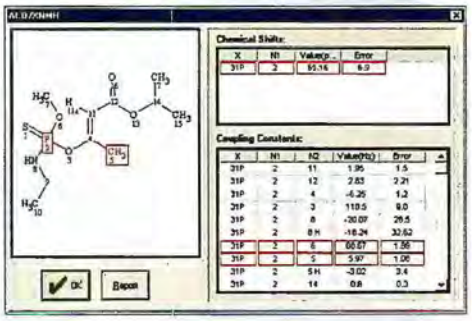
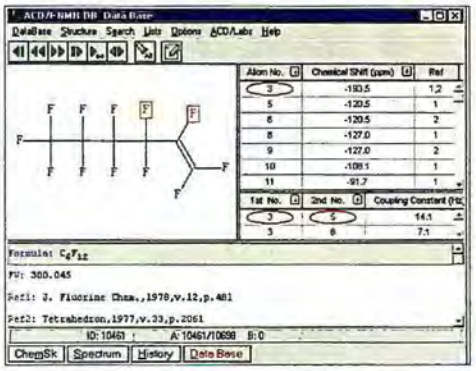
- ^{31}P NMR spectra for over 18,500 structures with over 23,300 chemical shifts and 8,600 coupling constants.

Each database includes original literature references, molecular formula, molecular weight and IUPAC names which can be searched and viewed. Search capabilities also include structure and substructure, and searching by exact value or range of values for chemical shifts and coupling constants.

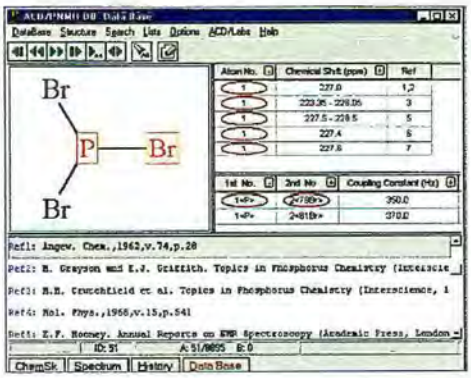


Display the predicted structure, interactively related to assigned shifts & coupling constants



Phosphorus database window showing chemical shifts, coupling constants, references, formula and IUPAC name

Fluorine Database window showing chemical shifts, coupling constants & references



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CENTRO DE INVESTIGACION Y DE ESTUDIOS AVANZADOS DEL I.P.N.

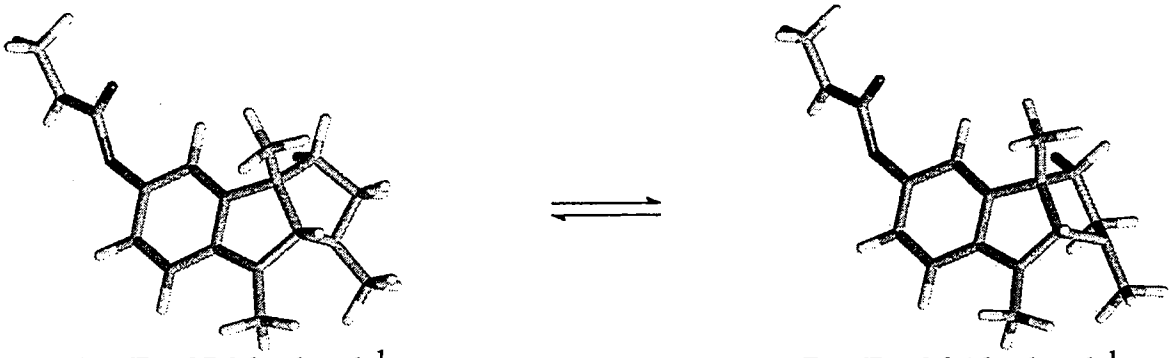
November 6, 2000
(received 11/20/2000)

Dr. Bernard L. Shapiro
Editor/Publisher
The NMR Newsletter
966 Elsinore Ct.
Palo Alto, CA 94303 USA

Conformational Study of Physostigmine

Dear Dr. Shapiro:

The conformational preference of physostigmine (**1**) in solution was investigated using ^{1}H NMR spectroscopy combined with a molecular mechanics study. This compound exists as two equilibrating conformations and the signals in the NMR spectrum are due to the average-weighted conformations (provided exchange is fast on the NMR time scale). Based on a comparison of dihedral angles (ϕ) measured from PCMODEL-optimized structures **A** and **B** with the experimentally-derived values, the NMR spectrum indicates the presence of mainly the **A** form with the H2β in a quasi-axial position (Table). Conformer **B** corresponds to a geometry in which the H2β is in a quasi-equatorial position.



A E = 37.2 kcal mol^{-1} **B** E = 36.4 kcal mol^{-1}

In the 300 MHz ^{1}H NMR spectrum of **1** in CD_2Cl_2 solution it was possible to perfectly discern the signals for every proton (Fig.). The pyrrolidine ring shows for H2α and H2β two close doublet of doublet of doublets (δ = 2.69 and 2.59 ppm) which were unambiguously assigned from a long-range W coupling. Thus, the H2β resonance (δ = 2.59 ppm) showed a four bond coupling with the signal at 4.10 ppm owing to H8aβ. Although the transitions of H3α and H3β (δ = 1.92 and 1.89 ppm) displayed some overlap and a low degree of degeneracy, they could be analyzed as first-order peaks. The shifts and coupling constants of each methylene proton were extracted from the spectrum and used as starting values in computer simulation of the spectrum. An iterative approach to improve agreement was

adopted. Using a generalized Karplus-type equation[1] dihedral angles (ϕ) were estimated. The X-ray crystallographic data[2] were the basis for identifying two low-energy conformers about C2-C3, and further refinement of each structure was then achieved, **B** being the most stable only by 0.8 kcal mol^{-1}.

Table. Calculated and observed dihedral angles (ϕ, °) and vicinal coupling constants (*J*, Hz) of **1**.

H–C2–C3–H	Conformer **A**		Conformer **B**		0.77 **A** + 0.23 **B**[a]		**1** (CD_2Cl_2)	
	ϕ	*J*	ϕ	*J*	ϕ	*J*	ϕ	*J*
2α3α	37.0	7.5	-44.4	5.5	40	7.0	40	6.9
2α3β	-83.2	0.4	-164.7	12.1	-57	3.1	-53	3.8
2β3α	159.3	11.5	78.4	0.6	144	9.0	144	8.9
2β3β	39.1	6.5	-41.1	6.8	38	6.6	40	6.2

[a] Average-weighted conformations.

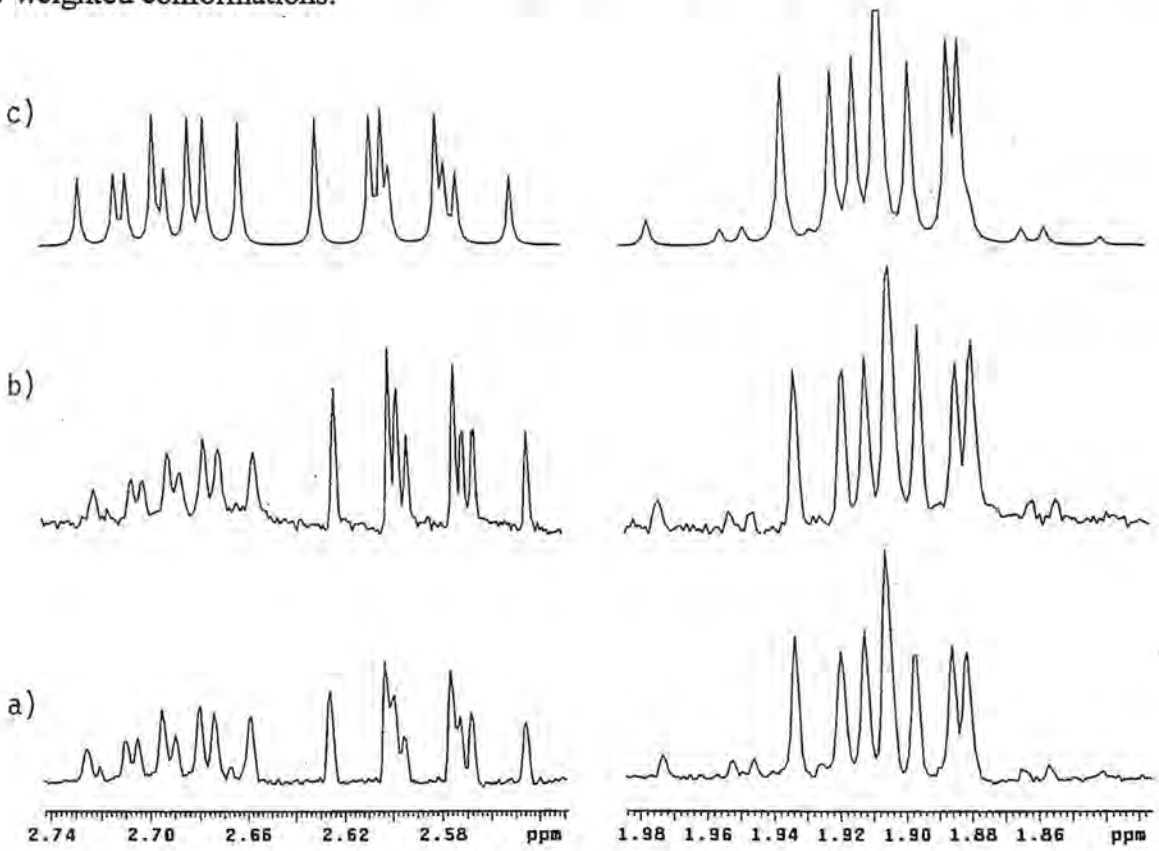


Figure . Methylene region of the ^{1}H NMR spectrum of **1**: a) experimental; b) H8a decoupled c) LAOCN3 simulated. The H8a transition was not included in the spectral simulation.

1. Cerda-García-Rojas, C.M., Zepeda, L.G. and Joseph-Nathan P. *Tetrahedron Comp. Methodol.* **1990**, *3*, 113.
2. Pauling, P. and Petcher, T.J. *J. Chem. Soc. Perkin Trans II*, **1973**, 1342.

Sincerely yours,

Martha S. Morales-Ríos
Norma F. Santos Sánchez
Pedro Joseph-Nathan
pjoseph@nathan.chem.cinvestav.mx

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(received 12/4/2000)

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

Alternate Uses of LC NMR Techniques

Dear Barry:

We have recently been collecting ^{13}C data for polymer microstructure investigations directly from the polymerization solutions that utilize non-deuterated solvent. The experimental acquistion times for these experiments ranged from 16 to 24 hours. While the actively shielded 11.7 T Oxford magnet we have has a slow drift rate, it is enough that over the period of time used to collect the data, details of the polymer microstructure become obscured due to line broadening associated with magnet drift.

While it is possible to overcome the magnet drift problem by collecting data in 1 hour increments, the real problem occurs when 'adding' the fids or spectra back together after all the data has been collected. The solution that Varian offers is to allow shifting the data in the spectra via the lsfreq command. Use of this command is possible in a macro, but it basically assumes that the drift rate is constant over the time of the experiment. Also it requires adding spectra rather than fids. We thought this approach was cumbersome to routinely implement so we opted for an approach used by the LC NMR folks.

The LC NMR community commonly employs solvent suppression during the LC run; furthermore, with the solvent gradients used in reverse phase chromatography, it is important to constantly monitor the position of the solvent signals so that they can be suppressed by presaturation or WET. Approaches such as these involve collecting a single scan on the solution and then determining the position of the solvent lines. After the position of the solvent lines has been determined, the suppression sequence is setup and the data acquired. The process is repeated at regular intervals.

We decided to utilize this approach to track the position of one of the solvent lines. Prior to actually collecting any data, we would obtain a 1 scan spectrum of the solution. We calculate the position of one of the lines in the solvent relative to the transmitter. We then store this information in one of the 'r' variables. We then setup the experiment to take data in approximately 1 hour increments [the period we determined that the magnet drift did not compromise the required resolution] for 16 to 20 hours. The spectrometer would then acquire an hour's worth of data and store it to disk. It would then acquire another scan of the solvent, calculate the position of the solvent line relative to the transmitter, compare this frequency to the stored frequency and if necessary move the transmitter so that the solvent was at the same position in the spectrum. Once it had done this, the spectrometer would collect data for another hour and repeat the process.

At the end of the total acquistion time, we would add the fids together to get a single fid for processing. Figure 1 shows the stability of data collected in such a manner.

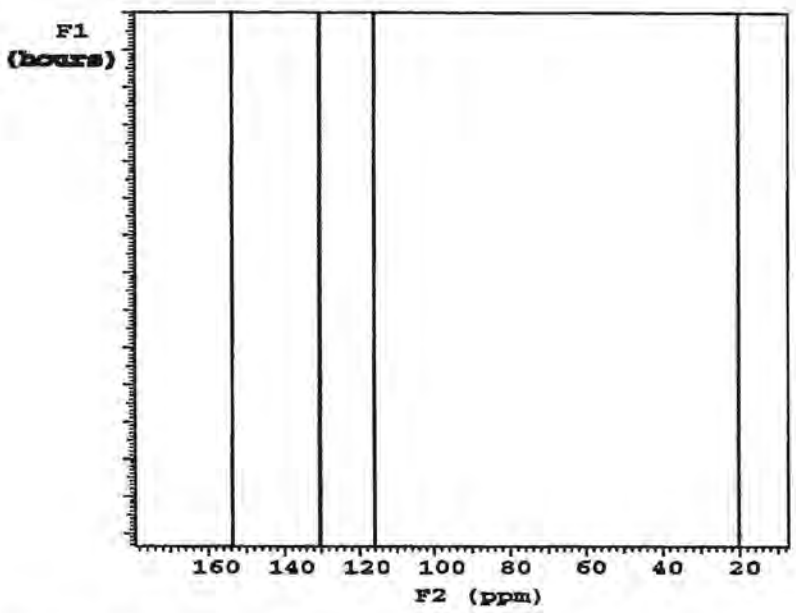

Figure 1. Pseudo 2D plot with the ^{13}C in f2 and time as f1. Data collected using LC NMR methodology as described above.

Figure 2 shows an expansion of the carbonyl region which clearly indicates that using this technique it is possible to use this approach to determine polymer microstructure in solvents where it is not possible to lock the magnet.

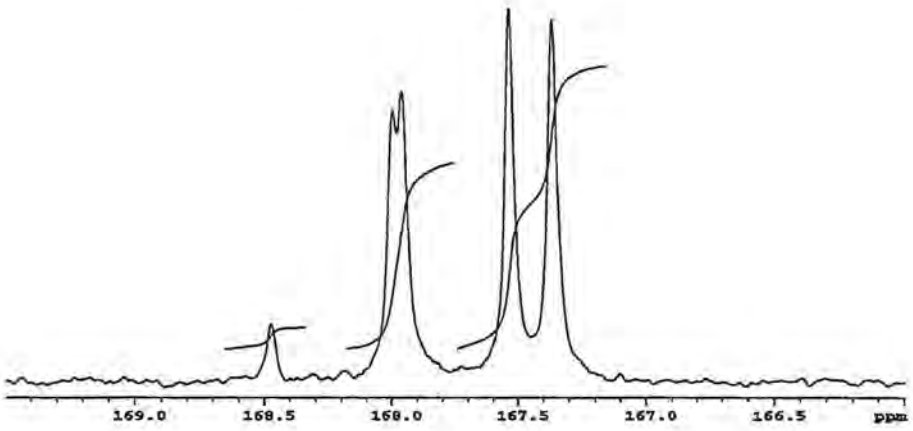

Figure 2 - ^{13}C carbonyl region after co-adding 16 fids. Each fid represents approximately 1hour of spectrometer time.

Please credit this contribution to the account of D.C. Roe.

Al Beeler Ashly Burri Alan English Laurie Galya

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November 30th 2000

(received 11/30/2000)

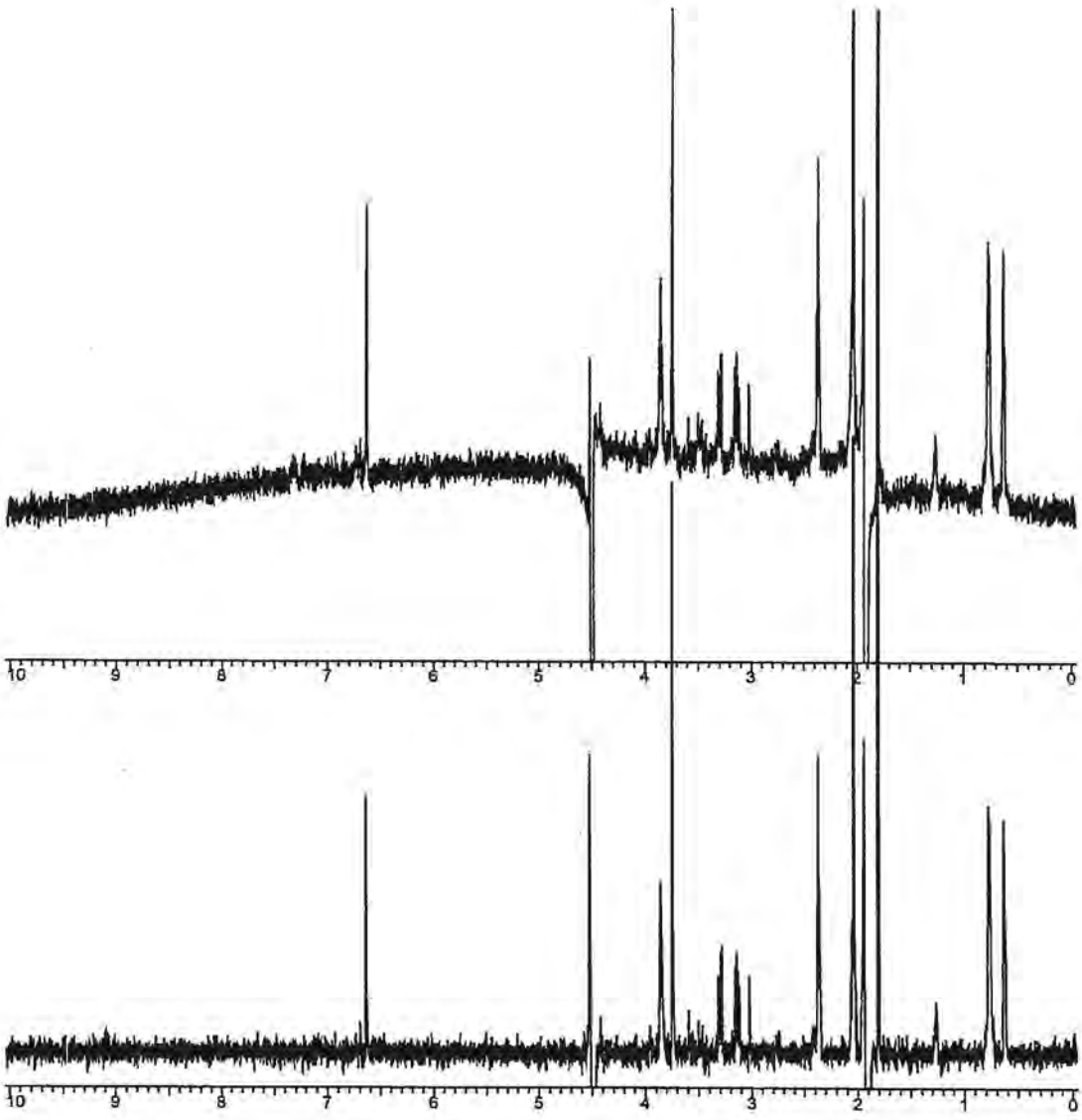
Dear Barry,

Nowadays hundreds of NMR spectra are generated on a daily basis in automation using NMR equipment provided in walk-up environments. It is common for the data analysis to require accurate integrations for quantitation purposes and this requires high quality spectra be generated prior to automated analysis. Among the sources of the error in any quantitative measurements in NMR spectra are distorted baselines which can arise due to the "dead time" problem of pulsed NMR, non-linearity of the filter phase response, the discrete nature of the Fourier transform, instrumental instabilities and other miscellaneous reasons. Often these problems are more extreme for spectra acquired in an LC-NMR run or at low concentrations since solvent suppression commonly has to be applied. Although some baseline problems can be avoided by adjusting acquisition parameters during the run-time of the NMR experiment and exploiting digital filtering and oversampling, post processing data treatment offers a more general way of correcting baseline distortions. Most popular approaches include reconstruction of the first points of the fid and approximation of the baseline in the frequency domain using Fourier series, polynomials and functions of special form. On the other hand, the majority of NMR desktop software allows the user to manually set the points belonging to the baseline and interpolate between them using analytical functions to completely model the baseline. 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 automated 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 poor recognition of the baseline.

In our efforts to optimize capabilities for the diverse needs of NMR spectroscopists who "want-it-all" in a desktop NMR processing package, it has become obvious that one of the more tedious tasks in processing NMR data from small samples is that spectra acquired utilizing solvent suppression generally require baseline correction. Preferably this baseline correction can be performed without manual intervention. Our recent developments in regards to baseline correction have been reported elsewhere (*Journal of Magnetic Resonance*, **146**, 122-125 (2000)). One of our baseline correction methods which we term *Spectrum Averaging* offers one possible avenue to deal with these baseline distortion issues.

To illustrate the utility of this powerful baseline correction method we show the results of its application to LC-NMR data of a metabolite, a glutathione adduct of an anti-viral compound, in Figure 1. The quality of the correction should be obvious especially the manner by which it deals with the dispersive response of the residual solvent resonance.

We are presently investigating the benefits of such a baseline correction procedure applied in automation to metabonomics data. For metabonomics generally a series of spectra are acquired under similar conditions in order to perform a NMR pattern recognition toxicity screen. Since these screens can often be comprised of several hundred samples any additional automation steps which reduce the need for manual processing can mean a significant improvement in throughput. The metabonomics approach utilizes Principal Components Analysis (PCA) on the histograms generated from urine spectra and it is critical that processing therefore be consistent as well as automated since the need to manually correct the baseline of all the spectra to obtain good integration is contrary to these objectives. Our examinations to date suggest that this baseline correction method is a significant step towards this end.



Yours sincerely,

Antony Williams, Eugene Vodopianov, Sergey Golotvin
Advanced Chemistry Development

John Shockcor
Dupont Pharmaceuticals

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Tel: (416) 368-3435 Toll-Free: 1-800-304-3988 Fax: (416) 368-5596

The NMR Newsletter - Book Reviews

Book Review Editor: István Pelczer, Dept. of Chemistry, Princeton University, Princeton, NJ 08544

"NMR Spectra of Polymers and Polymer Additives"

by

Anita J. Brandolini and Debora D. Hills

Marcel Dekker (http://www.dekker.com), New York, 2000,
ISBN 0-8247-8970-9, 634 pages, $195.00

Brandolini and Hills have put together a series of chapters designed to help all who are involved with the NMR spectroscopy of polymers. This book is an outstanding compendium that can certainly be included among the best NMR reference guides. It has all the relevant ingredients one could desire from a very extensive collection of standard NMR spectra of polymers and polymer additives: chemical shift assignments associated with molecular structure, practical experimental information and the most important applications. This exceptional approach distinguishes this publication from some others of this nature, and provides useful information either for NMR specialists who need to know about spectral characteristics of polymers, or for polymer scientists who may not be familiar with subtleties of NMR.

The book consists of a preface, ten chapters on 634 pages, four appendices on an additional 32 pages, six pages of index and 320 references. It presents 372 multinuclear liquid state NMR spectra (^{1}H, ^{13}C, ^{19}F, ^{29}Si, ^{27}Al, ^{31}P) of polymers, copolymers, blends and polymer additives, obtained at 9.4T. The introduction briefly explains important aspects of both polymer science and the principles of NMR spectroscopy. It gives an overview of the structure-property relations, the main polymerization reactions and discusses the most important features for the understanding of the chemical and physical properties of polymers. Still in the introduction, the authors present, in a very simplified way, some topics of basic NMR theory like chemical shifts, dipolar and scalar couplings, relaxation and the nuclear Overhauser effect – all important for the acquisition and interpretation of polymer spectra. Practical considerations, such as sample preparation and instrumental conditions for acquisition of quantitative ^{1}H and ^{13}C NMR spectra, are also emphasized.

The following individual chapters consist of a collection of NMR spectra (mostly ^{13}C and occasionally ^{1}H or other heteronuclei) of many different, commercially available polymers, and those of some interesting newer polymers, organized into categories according to the backbone structure of the molecules. Each chapter is preceded by a brief introduction, including information about sample handling, spectral interpretation, quantitative analysis and literature references. Also presented are the chemical structure, table of assignments, and experimental acquisition parameters. In addition there are summaries of the most common applications of the material, and attention drawn to the most important features to be observed in the spectra.

Chapter II considers the polymers containing aliphatic pendant groups produced from ethylene and propylene monomers. There are seventy ^{13}C and ^{1}H NMR spectra of linear, branched, high and low density polyethylenes, as well as copolymers of ethylene with many different olefins and other monomers. Spectra of polypropylenes with different tacticities, polymers and copolymers of other 1-olefins are presented.

continued

Polystyrene and its copolymers are the subjects of Chapter III, and in Chapter IV, spectra of vinyl esters, acrylic acid and esters, and α-substituted acrylate polymers are shown.

Chapters V, VI and VII present ^{13}C, ^{1}H and ^{19}F NMR spectra of polymers that contain aliphatic backbones with various miscellaneous side groups, polydienes and ether backbones, respectively. Chapter V presents a number of spectra illustrating how fluorine coupling patterns are sensitive to the polymer structure and its substituents. Chapter VI is largely dedicated to show the usefulness of the ^{13}C and ^{1}H resonances as analytical tools to identify the configuration of multiple isomers, including examples of many commercially important elastomers. Chapter VII provides an extensive ^{13}C spectrum collection of cellulose derivatives, emphasizing chemical shift effects of different substituents. It also refers to some quantitative NMR methods used to determine the molecular weight of several linear polyethers.

Chapter VIII shows ^{13}C and ^{1}H NMR spectra of thirty of the most common and important aromatic and aliphatic esters and polyamides. In addition to ^{13}C and ^{1}H spectra, Chapter IX collects ^{29}Si and ^{31}P spectra of polymers with distinct side chain groups. The majority of these spectra refer to the family of polysiloxane compounds, but other materials, such as polyurethane elastomers, polymers with sulfur-containing backbones, and polyphosphazenes are also included. Chapter X presents a variety of polymer additives, which are compounded into base resins at concentrations ranging from a few parts-per-million to several percent. This chapter includes some of most important and most frequently used additives that can be readily observed by NMR; fifty-four spectra of (aliphatic, unsaturated, aromatic) esters and phosphorus-containing additives are presented.

Appendix 1 lists major end-use applications for many of the polymers presented in chapters II to X. Appendix 2 contains some graphical summaries of ^{13}C chemical shifts for common polymers divided into categories such as polyolefins, vinyl polymers, polyesters and so on. Appendix 3 provides a comprehensive and up-to-date list of polymer suppliers and polymer additives in the US.

We strongly recommend this book as an excellent practical resource for the study of polymers and polymer additives for students, industry researchers and polymer scientists.

Dellyo R. Alvares
Naira M. da Silva
Sonia M. C. de Menezes*

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THE UNIVERSITY OF MANITOBA

DEPARTMENT OF CHEMISTRY WINNIPEG, CANADA

March 12, 1970

Dr. B. Shapiro
Chemistry Department
Texas A & M University
College Station, Texas 77843

Dear Barry,

Short title: A bit of doggerel looking for a good tune.
or Excerpts from the waist land.

You bother me with letters blue,[1)]
Imply that I will come to rue
My tardiness in writing you
About our doings fine and new.

You try to wake my cogitation!
Remembering that T_1 relaxation
Depends on robust stimulation
Of Schaefer, sunk in dissipation?

Before your final letter red
Comes to say that you are fed
Up with such a slug-a-bed,
Here is my missive to be read:

We did offer methyl nitrate
To other molecules as bait
To see if we could separate
Effects of friction [2)] on the fate
Of azote's [3)] level-jumping rate
From other causes [4)] known to date.

Our line-shape fits[5)] are going well,
But 'tis too early sure to tell
If Binsch's way of fitting many
Is better than Anet's uncanny
Peaking of the Gaussian bell.

If halogens nasty present their derrieres[6]
Single bonds and their rotational barriers
Cannot be found via M.O. carriers.
It behooves us therefore to play with a function
Which allows us to fit with empirical unction
The experimental to the calculational junction.
We have played this game with some success:
With halogen-toluenes we managed to guess
The stable conformers with some finesse.

When amino protons are hydrogen bonded
To neighbouring groups which are properly ronded,
They don't do what we thought they do
But hop between atoms with much ado [7]
It seems they shouldn't
And we wish they couldn't
But wait pro tem
It's in Can. J. Chem.

Christine and Helen, Rod and Fred
Brian and Jim and Mark have led
In doing the work to earn their bread.

Notes

1) My admiration knows no bounds
For editors and other hounds
Who dutifully do their rounds
With prods and threats and other sounds.

2) Aye, there's the rub
For Scholar Lehn and sub
Have partly scooped us from this tub.

3) This word is used in comprehension
That firm and constant use-abstention
Of simple words is a convention.

4) Causes have effects
And effects causes
But poetry elects
To have these clauses.

5) If you want the elocution
Of the compounds' appelution,
See our recent contribution
To this journal's page pollution.

6) My apologies to French Canadians
Whose amour propre is here invadians.

7) About nothing, of course.

Yours hopefully,

Ted Schaefer
Professor

TS/lg

P.S. Has anybody a 12 inch current stabilized magnet on offer? A nice old fashioned high impedance Varian magnet would do nicely.

Professor Schaefer was a loyal supporter of *The NMR Newsletter* in all its incarnations for over 30 years, until his recent retirement. He worked extensively on long-range proton-proton coupling constants and on solvent effects, *inter alia*. He probably no longer needs a 12" magnet.

BLS.

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.

IXth International Symposium on Magnetic Resonance in Colloid and Interface Science, St. Petersburg, Russia, **June 26-30, 2001**. Contact: Mrs. L. Ya. Startseva, Secretariat of ISMRCIS, Boreskov Institute of Catalysis, 5, Prosp. Akad. Lavrentieva, Novosibirsk, 630090, Russia. Tel: +7 (3832) 34-12-97; Fax: +7 (3832) 34-30-56; E-mail: star@catalysis.nsk.su.

Royal Society of Chemistry: 15th International Meeting on NMR Spectroscopy, Durham, England, **July 8-12, 2001**; Contact: Mrs. Paula Whelan, The Royal Society of Chemistry, Burlington House, London W1J 0BA, England; tel: +44 (0) 207-437-8656; fax: +44 (0) 207-734-1227; Email: conferences@rsc.org\; Use the subject header '01NMR15'

ESR and Solid State NMR in High Magnetic Fields, Stuttgart, Germany, **July 22-26, 2001**. Contact: Prof. Hans Paus, 2 Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany. Tel: ++49-711-685-5223 or -5217; Fax: ++40-711-685-5285; E-mail: ampere2001@physik.uni-stuttgart.de.

ISMAR 2001, Jerusalem, Israel, **August 19-24, 2001**; See http://www.tau.ac.il/chemistry/ISMAR.html.

14th European Symposium on Polymer Spectroscopy, Dresden, Germany, **September 2-5, 2001**. Contact: Institut für Polymerforschung Dresden e. V., ESOPS 14, Postfach 12 04 11, 01005 Dresden, Germany. Tel: +49 351 4658-282; Fax: +49 351-4658-214; E-mail: espos@ipfdd.de.

Fourth International Conference on Molecular Structural Biology, Vienna, Austria, **September 5-9, 2001**. Contact: Andreas Kungl, Austrian Chemical Society (GÖCH), Biochemistry Subgroup, c/o Institute of Pharmaceutical Chemistry, Univeristy of Graz, Universitätsplatz 1, A-8010 Graz, Austria. Tel: +43 316 380 5373; Fax: +43 316 382541; E-mail: andreas.kungl@kfunigraz.ac.at.

2nd Alpine Conference on Solid-State NMR, Chamonix-Mont Blanc, France, **September 9-13, 2001**; Contact: Alpine Conference Secretariat, Laboratoire STIM, Ecole Normale Supérieure de Lyon, 46 allée d'Italie, 69364 Lyon Cedex 7, France; alpine.SSNMR@ens-lyon.fr; Tel. +33-(0)4 72-72-84-86/ 83 84; Fax. +33 (0)4 72 72 84 83; http://ens-lyon.fr/STIM/alpineweb,html

XXth International Conference on Magnetic Resonance in Biological Systems, Toronto, Ont., **August 25-30, 2002**. For further information check www.uwo.ca/chem/icmrbs/, or contact: mgordon@julian.uwo.ca

Additional listings of meetings, etc., are invited.

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650-493-5971* - *Please call only between 8:00 am and 10:00 pm, Pacific Coast time.*

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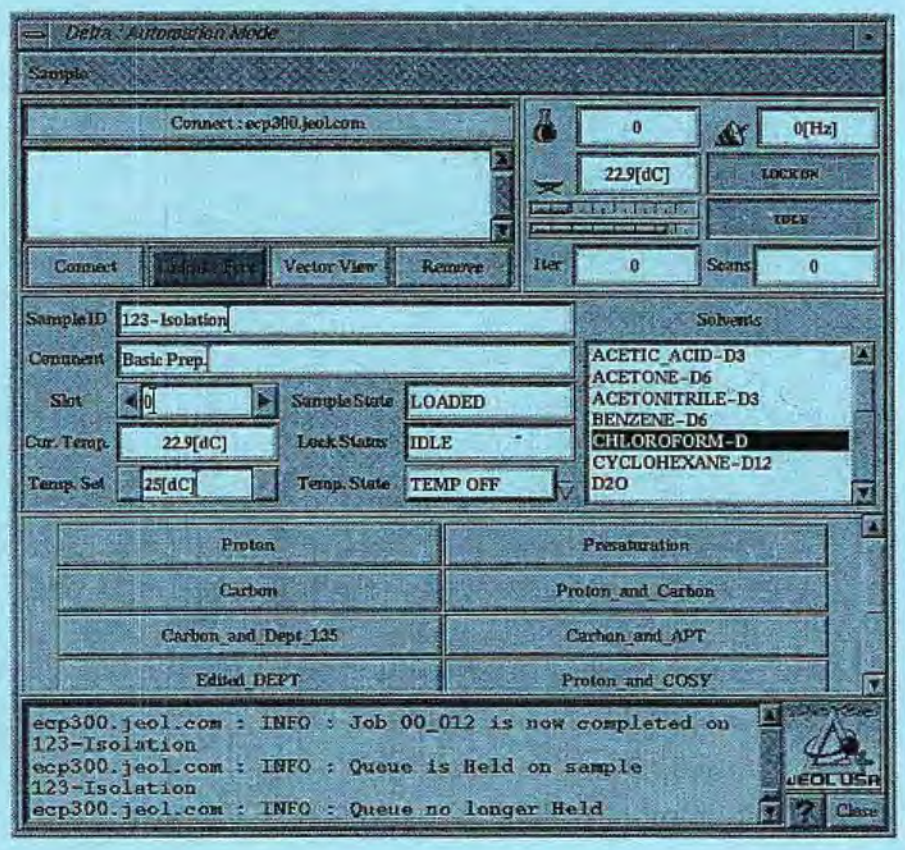

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