Network Printing                                Ellena, J.  2
Solid State NMR Spectroscopic Studies of the Thiourea Inclusions Compounds of the Two
Isomers of Methyl 4-t-Butylcyclohexanecarboxylate  Peters, J. A., and van Bekkum, H.  5
Position Available                               Stockman, B. J.  6
Comparison of $^1$H, $^{15}$N HSQC Spectra for Stromelysin in Free and Bound State  Li, Y.-C., and Gonnella, N. C.  9
Book Review ("Magnetic Resonance Imaging in Food Science" by B. Hills)  McCarthy, M. J.  13
Thinking Again About Time-Cubed Decays          Conradi, M. S., and McDowell, A. F.  17
7th Annual "Advances in NMR Applications" Symposium  Bishop, K./Nalorac Corp.  18
Tuning and Matching or Stay Tuned and Matched    Vuister, G. W., and van Os, J.  21
$^{59}$Co, $^{13}$C Dipolar Coupling                 Köhler, F. H., and Heise, H.  22
Pulsed NMR Sample Tubes                         Sullivan, M.  27
International School of Structural Biology and Magnetic Resonance, 4th Course: Dynamics,
Structure and Function of Biological Macromolecules; Erice, Sicily, Italy; May 25-June5, 1999  Jardetzky, O., and Lefèvre, J.-F.  28
Expanded Production Capacity for $^{13}$C and $^{18}$O  Saarinen, T./ISOTEC Inc.  30
Positions Available                              Botto, R. E.  35
Position Available                              Alam, T. M.  35
Another Blast from the Past                      Wertz, J. E.  36

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.

These restrictions and policies apply equally to both the actual Newsletter recipient/participants and to all others who are allowed access to the Newsletter issues. Strict adherence to this policy is considered essential to the successful continuation of the Newsletter as an informal medium for the exchange of NMR-related information.
NEW! Math functions for automated analysis

Macros can measure integrals and calculate results such as
- weight %
- mole fraction
- impurity levels

Totally automated!

The new macro commands function as an RPN-type calculator, with
- multiple memory locations
- add, subtract, multiply, divide, reciprocal, exponential, log
- 10-entry “stack”

Other macro commands have been added to:
- prompt for user input at runtime
- automatically measure integrals of preset regions
- output calculated values as text annotation on the spectrum

The spectrum below was generated with a single command, from FID to plot, including calculations and annotations

Mole % Impurity #1 = 9.378054
Mole % Impurity #2 = 1.926528
## AUTHOR INDEX

<table>
<thead>
<tr>
<th>Author</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alam, T. M.</td>
<td>35</td>
</tr>
<tr>
<td>van Bekkum, H.</td>
<td>5</td>
</tr>
<tr>
<td>Bishop, K.</td>
<td>18</td>
</tr>
<tr>
<td>Botto, R. E.</td>
<td>35</td>
</tr>
<tr>
<td>Conradi, M. S.</td>
<td>17</td>
</tr>
<tr>
<td>Ellena, J.</td>
<td>2</td>
</tr>
<tr>
<td>Gonnella, N. C.</td>
<td>9</td>
</tr>
<tr>
<td>Heise, H.</td>
<td>22</td>
</tr>
<tr>
<td>Hills, B.</td>
<td>13</td>
</tr>
<tr>
<td>ISOTEC Inc.</td>
<td>30</td>
</tr>
<tr>
<td>Jardetzky, O.</td>
<td>28</td>
</tr>
<tr>
<td>Köhler, F. H.</td>
<td>22</td>
</tr>
<tr>
<td>Lefèvre, J.-F.</td>
<td>28</td>
</tr>
<tr>
<td>Li, Y.-C.</td>
<td>9</td>
</tr>
<tr>
<td>McCarthy, M. J.</td>
<td>13</td>
</tr>
<tr>
<td>McDowell, A. F.</td>
<td>17</td>
</tr>
<tr>
<td>Nalorac Corp.</td>
<td>18</td>
</tr>
<tr>
<td>Peters, J. A.</td>
<td>5</td>
</tr>
<tr>
<td>Saarinen, T.</td>
<td>30</td>
</tr>
<tr>
<td>Stockman, B. J.</td>
<td>6</td>
</tr>
<tr>
<td>Sullivan, M.</td>
<td>27</td>
</tr>
<tr>
<td>van Os, J.</td>
<td>21</td>
</tr>
<tr>
<td>Wertz, J. E.</td>
<td>36</td>
</tr>
</tbody>
</table>

## ADVERTISER INDEX

<table>
<thead>
<tr>
<th>Advertiser</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acorn NMR, Inc.</td>
<td>inside front cover</td>
</tr>
<tr>
<td>Advanced Chemistry Development, Inc.</td>
<td>11</td>
</tr>
<tr>
<td>AMT</td>
<td>7</td>
</tr>
<tr>
<td>Bruker Instruments, Inc.</td>
<td>15</td>
</tr>
<tr>
<td>Cambridge Isotope Laboratories, Inc.</td>
<td>33</td>
</tr>
<tr>
<td>Isotec Inc.</td>
<td>23</td>
</tr>
<tr>
<td>MR Resources, Inc.</td>
<td>outside back cover</td>
</tr>
<tr>
<td>Oxford Instruments, Ltd.</td>
<td>3</td>
</tr>
<tr>
<td>Varian NMR Instruments</td>
<td>19</td>
</tr>
<tr>
<td>Voltronics Corporation</td>
<td>29</td>
</tr>
<tr>
<td>Wilmad Glass Company, Inc.</td>
<td>25</td>
</tr>
</tbody>
</table>

## SPONSORS OF THE NMR NEWSLETTER

- Abbott Laboratories
- Advanced Chemistry Development, Inc.
- Aldrich Chemical Company, Inc.
- AMT
- Amgen, Inc.
- Anasazi Instruments, Inc.
- Astra AB
- Bruker Instruments, Inc.
- Cambridge Isotope Laboratories
- Cryomag Services, Inc.
- The Dow Chemical Company
- E. I. du Pont de Nemours & Company
- Hewlett-Packard Company
- Isotec Inc.
- JEOL (U.S.A.) Inc., Analytical Instruments Division
- The Lilly Research Laboratories, Eli Lilly & Company
- Merck Research Laboratories
- Nalorac Corporation
- Oxford Instruments
- Pharmacia & Upjohn, Inc.
- Programmed Test Sources, Inc.
- SINTEF Unimrd MR Center, Trondheim, Norway
- Tecmag
- Unilever Research
- Union Carbide Corporation
- Varian NMR Instruments
- Zeneca Inc.

## 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 482, 18.

**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) 989-4573; 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 15235-8503; 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://mcmsg4.ch.man.ac.uk/mcmr/RF.html; fax: c/o M.H. Levitt +46-8-15 2187; email: mhl@physc.su.se.

**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; Email: enc@enc-conference.org.

**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.

*continued on inside back cover*
Network Printing

Dear Dr. Shapiro:

Multiple user NMR labs typically have several computers and must provide print services from most or all of these. The cost effective way to meet this need is to attach printers to the same network that is used for communication among computers. In our case as in most cases an ethernet-based network is available. Our NMR lab consists of four spectrometers, two are run by Sun workstations and the other two by PowerMacs. Additionally the lab contains two Unix workstations, and several Macintosh and IBM PC compatible computers. The user population is approximately 80. Our printing needs are met by two Hewlett Packard LaserJet printers, a 4M Plus and a 4000N. Each of the printers contains a HP JetDirect print server, a device which allows one to connect the printer directly to the network and complete print jobs from a wide array of computers including Mac, PC, and Unix machines. The JetDirect print servers may be configured directly from the front panel of the printer or remotely by using HP JetAdmin software. Each printer has an ethernet address and can simultaneously handle print jobs from computers using IPX/SPX, AppleTalk, DLC/LLC, and TCP/IP network protocols. We found that the JetDirect print servers and the JetAdmin software were easy to install and set up. Once the JetDirect print servers are set up, installation of the remote printers is as easy as installing a local printer. We have used the LaserJets and JetDirect servers for many months to provide print service for machines using the following operating systems: SunOS, Solaris, MacOS, Win95, and WinNT. IRIX and AIX based systems can also be used if they have a functioning Line Printer Daemon (LPD) or if the Unix server which hosts the network print queue has LPD. In summary, we find that our HP printers with JetDirect servers are a versatile, low maintenance solution for network printing. For more info on HP printers and JetDirect servers see http://www.hp.com/cgi-bin/peripherals/pandi.pl and http://www.hp.com/net_printing/jetdirect/index.html, respectively.

Sincerely,

Jeff Ellena
800MHz together with a 63mm room temperature bore

Available only from OXFORD
the right technology

If it's proof you are looking for, here are just some of the reasons why Oxford Instruments remains the world's leading supplier for 800MHz NMR magnet systems.

The only manufacturer to offer the significant advantages of a 63mm diameter room temperature bore, providing:
- Intrinsically superior transverse homogeneity
- Greater bore volume to facilitate high power, state-of-the-art NMR probes

The only manufacturer to offer a choice of systems:
- 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...

Oxford Instruments
NMR Instruments
Old Station Way, Eynsham,
Witney, Oxfordshire OX8 1TL, England
Tel: +44 (0)1865 884500 Fax: +44 (0)1865 884501
## Specifications for Vertical Bore, High Resolution NMR Magnet Systems

<table>
<thead>
<tr>
<th>NMR Operating Frequency (MHz/1H)</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>54</td>
<td>54</td>
<td>54</td>
</tr>
<tr>
<td>Magnet Type (Standard or shielded)</td>
<td>Standard</td>
<td>Standard</td>
<td>Standard</td>
<td>Standard</td>
</tr>
<tr>
<td>Field Stability (Hz/hour 1H)</td>
<td>&lt;2</td>
<td>&lt;2</td>
<td>&lt;3</td>
<td>&lt;15</td>
</tr>
<tr>
<td>Axial 5 Gauss Stray Field Contour (Metres)</td>
<td>1.8</td>
<td>2.65</td>
<td>2.19</td>
<td>2.75</td>
</tr>
<tr>
<td>Radial 5 Gauss Stray Field Contour (Metres)</td>
<td>2.3</td>
<td>2.75</td>
<td>2.19</td>
<td>3.2</td>
</tr>
<tr>
<td>Cryostat Type</td>
<td>Compact TSFB</td>
<td>Compact TS</td>
<td>Compact TSFB</td>
<td>TSFB</td>
</tr>
<tr>
<td>Minimum Helium Refill Interval (Days)</td>
<td>50</td>
<td>235</td>
<td>120</td>
<td>183</td>
</tr>
<tr>
<td>Helium Refill Volume (Litres)</td>
<td>26</td>
<td>79</td>
<td>68</td>
<td>26</td>
</tr>
<tr>
<td>Year Hold Cryostat Option</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Nitrogen Refill Interval (Days)</td>
<td>14</td>
<td>14</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>Minimum Nitrogen Refill Volume (Litres)</td>
<td>90</td>
<td>51</td>
<td>51</td>
<td>90</td>
</tr>
<tr>
<td>* Minimum Operational Ceiling Height (Metres)</td>
<td>2.69</td>
<td>2.52</td>
<td>2.82</td>
<td>4.16</td>
</tr>
<tr>
<td>System Weight (kg) Including Cryogen's</td>
<td>120</td>
<td>315</td>
<td>391</td>
<td>120</td>
</tr>
</tbody>
</table>

### Room Temperature Shim Specifications

<table>
<thead>
<tr>
<th>Shim Type (Model)</th>
<th>Number of Channels</th>
<th>External Diameter (Cryostat Bore Size)</th>
<th>Internal Diameter (NMR Probe Diameter)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23/64/64</td>
<td>23</td>
<td>54mm</td>
<td>45mm</td>
</tr>
<tr>
<td>18/8/21/3</td>
<td>18</td>
<td>18mm</td>
<td>18mm</td>
</tr>
<tr>
<td>26/9/7/3</td>
<td>26</td>
<td>26mm</td>
<td>26mm</td>
</tr>
<tr>
<td>2/S/1/0</td>
<td>28</td>
<td>28mm</td>
<td>28mm</td>
</tr>
<tr>
<td>60/5/10</td>
<td>40</td>
<td>40mm</td>
<td>40mm</td>
</tr>
<tr>
<td>26/1/4/5</td>
<td>29</td>
<td>29mm</td>
<td>29mm</td>
</tr>
<tr>
<td>56/3/5</td>
<td>36</td>
<td>36mm</td>
<td>36mm</td>
</tr>
</tbody>
</table>

### Contact Information

**UK**
Oxford Instruments
NMR Instruments, Old Station Way
Enysham, Witney, Oxon, OX8 1TL
Tel: +44 (0)1865 884500
Fax: +44 (0)1865 884501
E-mail: info.nmr@oxinst.co.uk

**France**
Oxford Instruments SA
Parc Club-Orsay
Universite, 27, rue Jean Rostand, 91893 - Orsay Cedex, France
Tel: +33 1 6941 8990
Fax: +33 1 6941 8680
E-mail: info.nmr@oxinst.co.uk

**Germany**
Oxford Instruments GmbH
Kreuzberger Ring 38, Postfach 4509, D-6200 Wiesbaden, Germany
Tel: +49 611 76471
Fax: +49 611 764100

**Japan**
Oxford Instruments K.K.
Haseman Building, 201106 Tomioka, Tokyo, Japan 135
Tel: +81 3 5245 3261
Fax: +81 3 5245 4472
E-mail: oinmrwest@aol.com

**USA**
Oxford Instruments
NMR Instruments, 3120 Hansen Way, IWS D177, Palo Alto, CA 94304-1030, USA
Tel: +1 650 813 9068
Fax: +1 650 813 9069
E-mail: oinmrwest@aol.com


---

**Dimensions**

- External Diameter (Cryostat Bore Size): 54mm
- Internal Diameter (NMR Probe Diameter): 45mm
- External Diameter: 50mm
- Internal Diameter: 40mm
- External Diameter: 60mm
- Internal Diameter: 45mm
- External Diameter: 62mm
- Internal Diameter: 51mm

---

**UK**
Oxford Instruments
NMR Instruments, Old Station Way
Enysham, Witney, Oxon, OX8 1TL
Tel: +44 (0)1865 884500
Fax: +44 (0)1865 884501
E-mail: info.nmr@oxinst.co.uk

**France**
Oxford Instruments SA
Parc Club-Orsay
Universite, 27, rue Jean Rostand, 91893 - Orsay Cedex, France
Tel: +33 1 6941 8990
Fax: +33 1 6941 8680
E-mail: info.nmr@oxinst.co.uk

**Germany**
Oxford Instruments GmbH
Kreuzberger Ring 38, Postfach 4509, D-6200 Wiesbaden, Germany
Tel: +49 611 76471
Fax: +49 611 764100

**Japan**
Oxford Instruments K.K.
Haseman Building, 201106 Tomioka, Tokyo, Japan 135
Tel: +81 3 5245 3261
Fax: +81 3 5245 4472
E-mail: oinmrwest@aol.com

**USA**
Oxford Instruments
NMR Instruments, 3120 Hansen Way, IWS D177, Palo Alto, CA 94304-1030, USA
Tel: +1 650 813 9068
Fax: +1 650 813 9069
E-mail: oinmrwest@aol.com

---

Solid state NMR spectroscopic studies of the thiourea inclusion compounds of the two isomers of methyl 4-t-butylocyclohexanecarboxylate

Dear Dr. Shapiro,

One of us (HvB) was studying thiourea inclusion compounds of cyclohexane derivatives some 30 years ago.\(^1\) A recent publication on an NMR study of carboxylic acid guests in urea\(^2\) gave rise to some nostalgia and prompted us to dig up some of our old thiourea inclusion compounds and to run their \(^{13}\)C NMR spectra. It appeared that the compounds survived well and the spectra provided us with some new structural information. Here, we report on the \(^{13}\)C CP-MAS spectra of the thiourea inclusion compounds of the cis and trans isomers of methyl 4-t-butylocyclohexanecarboxylate (see Figure 1).

It is well known that thiourea forms crystalline inclusion compounds with suitable organic compounds. The host-guest compounds can be described as consisting of hexagonal honeycombs of thiourea surrounding channels with an internal diameter of about 7 \(\text{Å}\). Previously, X-ray diffraction (powder) showed that cis and trans methyl 4-t-butylocyclohexanecarboxylate have a repeat period of 10.7 and 12.3 \(\text{Å}\), respectively in the thiourea host.\(^1\) Since this corresponds well with the molecular dimensions of these compounds, it can be concluded that the guest molecules have head-tail stacking in the inclusion compounds.

The \(^{13}\)C chemical shifts of the esters in the inclusion compounds (see Figure 1) are close to those of the pure esters in a solution of CDCl\(_3\). This suggests that the chair conformation of the cyclohexane rings of these compounds is preserved upon inclusion in thiourea. Both the C-10 and the C-7 nuclei of the included trans ester show two resonances in the \(^{13}\)C NMR spectra, whereas the resonances for all other nuclei are not split and relatively sharp. Most likely, two different orientations of the guest molecules with respect to each other occur in the thiourea channels.

The line widths of the resonances of the thiourea adduct of the cis ester are much larger than those of the trans compound, indicating some mobility in the former. The line widths of the C-1, C-2,6, and C-10 are larger than those of the other resonances. This might be explained by exchange between two conformations of the COOCH\(_3\) moiety. It is known that the C=O function of esters groups prefers an eclipsed configuration with neighboring C-C bonds. For the cis ester this means that the C=O can be either eclipsed to C1-C2 or to C1-C6.

Sincerely,

Joop A. Peters

Herman van Bekkum
Figure 1. $^{13}$C CP MAS NMR spectra of the thiol retnia inclusion compounds of cis and trans methyl 4-tert-butylcyclohexane carboxylate. The carbonyl region is not shown.

References

Postdoctoral Position Available

I currently have an opening for a postdoctoral scientist in my lab in the Structural, Analytical & Medicinal Chemistry unit at Pharmacia & Upjohn in Kalamazoo, Michigan. The position will involve developing and applying flow NMR techniques to enhance and drive combinatorial chemistry and ligand-binding screening components of drug discovery research. The successful candidate will collaborate with scientists in chemical informatics and in structural, combinatorial and medicinal chemistry. Our facilities include fully-equipped 400, 500 and 600 MHz NMR spectrometers. Applicants should have a recent or soon-to-be-received Ph.D. in chemistry, biochemistry or a related field, with experience in biomolecular NMR spectroscopy. Applications should be sent directly to me at the address below. For more information, please contact:

Dr. Brian J. Stockman
Structural, Analytical & Medicinal Chemistry
7255-209-007
301 Henrietta St.
Kalamazoo, MI 49001
phone: 616-833-1882
e-mail: brian.j.stockman@am.pnu.com.
AMT is the leading supplier of solid state RF power amplifiers for NMR/NMRI.

ISO-9001 Certified

AMT amplifier products are designed specifically for NMR/NMRI applications. This means clean pulses and noise blanking fast enough for multi-pulse applications. AMT's products feature highly reliable technical solutions for producibility and reliability.

AMT's amplifiers cover frequencies from 6-500MHz, with power levels from 50 watts to 8 kilowatts. AMT products are just what you need for today's reality and tomorrow's challenges.

AMT
An Employee Owned Company
2570 E. Cerritos Avenue, Anaheim, CA. 92806
Tel: (714) 456-0777 • Toll Free: (888) 545-4AMT • Fax: (714) 456-0778 • www.amtinc.com
KEY AMPLIFIER FEATURES

♦ Dual mode operation for pulse and CW type signals

♦ Blanking delay time >1 µs for multi-pulse

♦ Linearity ±1 dB for shaped pulses

♦ CW power capability for decoupling

♦ Dual mode protection

♦ Duty cycle up to 10%

♦ Protection: Infinite VSWR at rated power
  Input overdrive
  Over duty cycle/pulse width
  Over temperature

♦ Reliable and safe to use
Comparison of $^1$H, $^{15}$N HSQC Spectra for Stromelysin in Free and Bound State

Dear Dr. Shapiro,

Recent studies with the catalytic domain of human stromelysin-1 (SLN) have led us to compare $^1$H, $^{15}$N HSQC spectra of this protein in the free and bound states. Figure 1 shows (A) the $^1$H, $^{15}$N HSQC spectrum of the stromelysin-CGS 27023 complex and (B) the $^1$H, $^{15}$N HSQC spectra of apo-stromelysin-1 overlaid with the spectrum of stromelysin-1 complexed to CGS-27023. Both spectra were acquired in buffer containing 20 mM Tris $\text{HCl}$, 20 mM CaCl$_2$, 0.02% NaN$_3$, 90% H$_2$O/10% D$_2$O, pH 6.8. Chemical shift assignments for the SLN-CGS 27023 complex have been made and the three dimensional structure has been determined (Y. Li, X. Zhang, R. Melton, V. Ganu & N.C. Gonnella, Biochemistry, in press.)

Visual inspection of the overlaid spectra clearly shows significant shifts of amide proton & nitrogen resonances for stromelysin bound to a potent inhibitor (nanomolar range) vs. the uninhibited protein. While many prominent shifts occurred at the binding site (example: Val 163, Leu 164, Ala 165, Leu 222, Tyr 223) other resonances more remote from the immediate binding site also experienced significant chemical shift changes (example: Trp 124, Ala 167, Asp 177, His 179, Thr 187, Arg 231, Ile 242). Hence, although it is expected that inhibitor binding would cause chemical shift changes at the catalytic binding site, we have observed that other areas more remote from the binding site were found to exhibit significant chemical shift changes in the absence of inhibitor.

These results indicate that changes in chemical shifts from $^1$H, $^{15}$N HSQC spectra may not always unambiguously or exclusively identify the binding site resonances for potent inhibitors. Such considerations need to be taken into account when using HSQC spectra to identify binding site regions especially when the 3-D structure of the protein is not known.

Sincerely,

Yu-Chin Li

Nina C. Gonnella
Figure 1. A) $^{15}$N, $^1$H HSQC of SLN-CGS 27023 complex. B) $^{15}$N, $^1$H HSQC of SLN-CGS 27023 complex overlaid with HSQC of free SLN. Some resonances remote from the binding site that shift upon inhibitor binding are displayed.
19F/31P NMR Predictors

ACD/NMR Predictors are able to calculate chemical shifts and where appropriate, coupling constants for a variety of chemical structures. The ACD/NMR prediction suite has expanded now to include 19F and 31P prediction capability. The programs utilize our proprietary prediction algorithms developed over a period of many years, in conjunction with internal databases of experimental data collected from the open literature and verified for quality by our compilation team.

Features of ACD/NMR Predictor

- Calculated chemical shifts are always provided with 95% confidence intervals so that you can always know the reliability of the calculated values
- Fully integrated with other ACD/NMR software
- Includes ACD/ChemSketch as an Integrated editor for drawing chemical structures and designing professional reports quickly and easily. This is a powerful molecular editor which allows automatic or customized numbering of molecules. Molecules, names, graphical objects, predicted spectra, and text which are displayed in ChemSketch can be cut and pasted into word processor programs.
- Calculates chemical shift tables based on internal DAT files with tens of thousands of experimental chemical shifts
- Manual or automatic numbering of atoms in molecules prior to prediction. Same atomic numbering schemes for all nuclei.
- Calculates the spin-spin interaction of carbon nuclei with magnetic nuclei of other elements, proceeding from the natural ratios of magnetic isotopes.
- Easily attributes chemical shifts, and coupling constants to nuclei and vice versa.

<table>
<thead>
<tr>
<th>NUCLEUS</th>
<th>STRUCTURES IN INTERNAL DB</th>
<th># CHEMICAL SHIFTS</th>
<th># COUPLING CONSTANTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>31P</td>
<td>18,500</td>
<td>25,000</td>
<td>8,000</td>
</tr>
<tr>
<td>19F</td>
<td>11,400</td>
<td>25,000</td>
<td>15,000</td>
</tr>
</tbody>
</table>

19F/31P NMR

Each database includes original literature references, molecular formula, molecular weight and IUPAC names which can be searched and viewed. All data have been collected from scientific literature and verified for quality by our database team.

Search capability also includes structure and substructure, and searching by molecular weight, molecular formula, chemical shifts, coupling constants and IUPAC name.

ACD/NMR DBs allow you to view chemical shifts and coupling constants for known compounds.

Phosphorus Database window showing chemical shifts, coupling constants, and references

Fluorine Database window showing chemical shifts, coupling constants, and references

See reverse side for contact information
2D NMR Processor

A simple-to-use interface that brings maximum 2D processing capabilities to the desktop. Fully integrated with our powerful structure drawing package, ACD/ChemSketch, NMR processing at the desktop has finally come of age.

ACD/2D NMR Processor allows you to:

- Import different spectrometer vendor formats;
- Carry out basic spectral manipulation such as Fourier Transform, weighting functions, phase correction, baseline correction, calibration, peak picking and integration;
- View magnitude spectrum, power spectrum and symmetrization;
- Display slices and 3D projections;
- Attach chemical structure and additional data to the spectrum;
- Attach 1D spectra to the spectrum;
- Print spectra and create reports using all the power of ACD/ChemSketch.

2D NMR Predictor

Calculate spectra of some 2D experiments: H,H COSY; C,C COSY (INADEQUATE); C,H COSY (HETCOR); H,H and C,H J-resolved. Display data as intensity or contour plots.

Additional features:
- View tables of shifts and coupling constants
- Possibility to correct chemical shift or coupling constant values and recalculate the spectrum

Optionally:
- Use direct or all coupling constants for C,C COSY and C,H J-resolved experiments
- Use 1J-3J constants or all coupling constants for H,H COSY and H,H J-resolved experiments
- Use first-order or higher-order interactions for prediction of the H,H J-resolved experiment
- Use heteronuclear couplings for all the experiments

Experimental & predicted H,H COSY spectra for strychnine
"Magnetic Resonance Imaging in Food Science

by

Brian Hills

John Wiley & Sons, Inc., New York, NY 10158; 1998;
ISBN 0-471-17087-9; 342 pages; $89.95 (cloth)

In the preface for his book, Brian Hills describes his goals as, "This book should be of value to all food scientists and technologists who seek a better understanding of the present and future role of MRI in their discipline, and conversely, to NMR and MRI specialists who wish to explore the potential of this wonderful technique in the arena of foods." The author has achieved his objectives with this book. Brian has done a fine job of describing the type of information needed for food processing studies and how MRI can provide that information. There is a good balance of basic food processing and engineering information as well as the 'how to use MRI' for obtaining the needed data to complete engineering models.

The book consists of thirteen chapters and a seven-page index. The thirteen chapters are divided into three sections based on distance scale (macroscopic, microscopic and molecular). The definition of what is a microscopic length scale is somewhat arbitrary and Brian uses a voxel with at least one dimension less than 40 µm. MRI studies with larger pixel dimensions are classified as macroscopic.

The initial section on macroscopic length scales begins with an introductory chapter on NMR/MRI. This chapter is written for individuals who have had a previous introduction to the basic theory of NMR. The breadth and impact potential of MRI studies is well covered in this section. The next three chapters deal with macroscopic behavior of food materials during mass transfer, phase changes, temperature measurement, quality and rheological behavior. The last four chapters in this section cover solid-imaging, process control, whole-plant functional imaging, and unconventional techniques.

The book's strength is in the final two sections where Brian has primarily done most of his research. These sections are particularly well written and insightful. The molecular origins of NMR relaxation phenomena are widely misunderstood in food science. Brian's work has greatly improved the understanding of the mechanisms controlling both transverse and longitudinal relaxation in foods. Chapters 12 and 13 should be required reading for researchers using relaxation times to correlate to a 'quality' parameter in a food or agricultural product.
The book though is not without some minor problems. Most of the reproduced images are of a slightly lower quality than the original published versions. Several of the references are repeated, for example numbers 124 and 183 are the same. Other references have been missed, such as, the work by L.D. Hall and myself on developing MRI as a viscometer. An additional disappointment with the references is the lack of consistent use of titles. Most references have titles included, which is very useful for the reader. It would also seem more appropriate to use one of Brian's own images of a food product for the cover illustration rather than the image of water around nylon fibers.

The goal of the book is to describe how to incorporate and use MRI to study foods and food processes. The book is not intended as a comprehensive review of food science literature or MRI applications to food science. We are now in a position to use MRI to rigorously test well-developed theoretical models of transport phenomena, which are in the literature. For example, the detailed theoretical and experimental study of drying apples by Crapiste, Whitaker and Rotstein is not mentioned in this book. In their study, they were able to validate their detailed microscopic cellular based mathematical model and by using their model one can calculate the contribution of different pathways for moisture transport (e.g. intercellular spaces, cell-to-cell, or cell wall-to-cell wall). The MRI techniques discussed in this book are precisely the experimental techniques needed to test assumptions in this mathematical model.


**Michael J. McCarthy**  
Food Science and Technology  
University of California  
One Shields Avenue  
Davis, CA 95616-8598

mjmccarthy@ucdavis.edu
Entering a New Frontier

700MHz/54mm Shielded Magnet

Bruker continues to be the world's leader in NMR magnet technology and is proud to introduce a new milestone: 700MHz actively shielded superconducting magnet. The 700 UltraShield™ is the first compact magnet system for Ultra-High Field NMR, which is easy to site in a standard NMR laboratory. This new magnet delivers the same excellent performance, which comes with every Bruker system. Its' design is based on Bruker's UltraShield technology, which has been successfully applied to other field strengths since 1996. You can now enjoy the benefits of Ultra-High Field NMR without being concerned with siting issues. In fact, the 700 UltraShield can be placed in a smaller space than previously required by a traditional 500MHz magnet!

UltraShield™ Magnet Series

UltraShield is an advanced self-shielding magnet technology developed by Bruker. The UltraShield magnet series is manufactured by our company located near Zurich, Switzerland. Our more than 30 years of experience in development and production of superconducting magnets enables us to deliver NMR magnets with exceptional performance and reliability. Many Bruker magnets built in the late 70's and early 80's are still on field, providing quality data and dependable service.

Main Features

- Active shielding technology strongly reduces stray fields and requires less lab space than a traditional 500MHz magnet.
- Advanced magnet design provides outstanding field homogeneity with excellent resolution and non-spinning lined shape.
- Optimized cryostat design allows easy handling and requires low ceiling height for installation and operation.
- Lowest drift rates.
- Special sensors connected to the Automatic Cooling Device (ACD) prevent stresses during magnet cooling.
- Advanced vibration isolation system integrated in the cryostat stand provides optimal dampening of ground vibrations.
- Electronic atmospheric pressure device stabilizes the field drift and helium boil-off when changes in atmospheric pressure occur (optional).
## SPECIFICATIONS

### MAGNET

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NMR Frequency ((^1)H)</td>
<td>700 MHz</td>
</tr>
<tr>
<td>Operating Field</td>
<td>16.45 Tesla</td>
</tr>
<tr>
<td>Field Stability (guaranteed value in persistent mode)</td>
<td>&lt; 10.5 Hz/hr</td>
</tr>
<tr>
<td>Cryoshims</td>
<td>Z, Z', Z'', X, Y, XZ, YZ, XY, X^2-Y^2</td>
</tr>
<tr>
<td>Axial Range with Field Homogeneity better than 10 ppm (w/o RT Shimming)</td>
<td>&lt; 2.50 m</td>
</tr>
<tr>
<td>5G Line from the Magnetic Center</td>
<td>&lt; 3.50 m</td>
</tr>
<tr>
<td>Resolution at 50%</td>
<td>&lt; 0.55 Hz</td>
</tr>
<tr>
<td>1% CHCl(_3) 5mm spinning Lineshape</td>
<td>&lt; 7 Hz*</td>
</tr>
<tr>
<td>1% CHCl(_3) 5mm non-spinning</td>
<td>&lt; 14 Hz*</td>
</tr>
<tr>
<td>Spinning Sidebands</td>
<td>&lt; 2%</td>
</tr>
</tbody>
</table>

*Typical values obtained with the BOSSII™ shim system.*

### CRYOSTAT

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Helium Evaporation Rate</td>
<td>~ 110 ml/hr</td>
</tr>
<tr>
<td>Helium Refill Volume</td>
<td>~ 315 liters</td>
</tr>
<tr>
<td>Helium Hold Time</td>
<td>&gt; 120 days</td>
</tr>
<tr>
<td>Nitrogen Evaporation Rate</td>
<td>~ 725 ml/hr</td>
</tr>
<tr>
<td>Nitrogen Refill Volume</td>
<td>~ 365 liters</td>
</tr>
<tr>
<td>Nitrogen Hold Time</td>
<td>&gt; 21 days</td>
</tr>
<tr>
<td>Weight Without Cryogens</td>
<td>2700 kg</td>
</tr>
<tr>
<td>Weight Including Cryogens</td>
<td>3200 kg</td>
</tr>
<tr>
<td>Minimum Ceiling Height (with Special Equipment)</td>
<td>3.60 m</td>
</tr>
<tr>
<td>Reduced Minimum Ceiling Height</td>
<td>3.45 m</td>
</tr>
</tbody>
</table>

---

**USA**

BRUKER INSTRUMENTS, INC.
BRUKER MAGNETICS
19 Fortune Dr., Manning Park
Billerica, Mass. 01821
Tel. (978) 667 - 9580
Fax. (978) 667 - 3954
E-mail: magnetics@bruker.com

USA

[http://www.bruker.com](http://www.bruker.com)

**Switzerland**

BRUKER AG
BRUKER MAGNETICS
Industriestrasse 26
CH-8117 Fallanden
Tel. (41) 1 825 91 11
Fax. (41) 1 825 96 96
E-mail: magnetics@bruker.ch

---

700MHz/54mm
UltraShield™ Magnet

Dimensions in millimeters unless stated otherwise
Dear Dr. Shapiro:

We have been playing with the well-known \( \exp(-bt^3) \) decay of spin echoes. Normally, this arises in the case of spins diffusing through a uniform gradient of magnetic field. Recently, such \( t^3 \) decays have been observed in incommensurately distorted solids; the interpretation has been given in terms of a diffusing modulation wave, coupling to the spin via quadrupole interaction.

All of this bring up the simple question: are there other circumstances in which the spin echo amplitude decays as \( \exp(-bt^3) \)? Our answer is 'yes'. Specifically, we consider a spin subjected to a slowly and continuously varying random field. Provided the random field has an exponential autocorrelation (fairly standard) and one works at times \( t \ll \tau_\text{c} \) (the correlation time of the fluctuating field; this is not a standard limit), it turns out that the \( t^3 \) echo amplitude decay will occur.

Now, in the old literature Klauder and P. W. Anderson\(^1\) have an analytical expression for both the FID and the echo amplitude for this case. Their expression becomes \( \exp(-bt^3) \) in the limit \( t \ll \tau_\text{c} \).

Now, does this occur in NMR (other than for spins diffusing through a gradient)? For a slowly varying interaction (recall \( t \ll \tau_\text{c} \) to result in substantial de-phasing, the interaction must be large. And the requirement that the field fluctuate continuously rules out the common examples wherein a given spin interacts with 4 or 8 nearest neighbor spins: when a spin \( S \) flips, there is a discontinuous change in \( S_z \). So NMR examples will be rare.

But there may be examples in NQR, where the NQR frequency can be substantially modulated by the disorder in the solid. If whatever causes the disorder is mobile, one may find a Gaussian-distributed, continuously varying interaction.

We welcome the thoughts and remarks of the readers.


Sincerely,

Mark S. Conradi

Andrew F. McDowell
Knox College
Department of Physics
Galesburg, IL 61401
You are invited to attend the

7th ANNUAL
ADVANCES IN NMR APPLICATIONS
SYMPOSIUM

Featuring the Latest Developments in Experimental Techniques

To be held prior to ENC at the
Omni Rosen Hotel
Grand Ballroom C
(located a short walk from the Clarion Plaza Hotel)

Sunday, February 28, 1999
1:00 to 6:00 p.m.

The agenda includes a presentation of recent results by leading
NMR experimentalists concerning applications of pulsed field
gradient and classical NMR techniques with both large and small
molecular systems.
The results obtained will be of interest to all liquid state NMR
spectroscopists.

Request a detailed program or RSVP by contacting
Kathy Bishop, Nalorac's ENC Coordinator

Transportation will be provided between the
Omni Rosen and Clarion Plaza Hotels

NALORAC
A CORPORATION OF CA MENTOR RESEARCH FOUNDATION
841-A Arnold Drive, Martinez, CA 94553
Phone: (925) 229-3501 Fax: (925) 229-1651
Email: kathy.bishop@nalorac.com
The Last Word in DSP
From the First Name in NMR

Real-Time DSP spectrum of SmM BPTI using Varian's Time-Corrected, Zero-Phase Digital Filters
Excellent baselines can be obtained with no baseline correction. The full spectrum is shown.

At Varian, DSP Means “Designed for Superior Performance”

Digital signal processing combines over-sampling and digital filtering to improve signal/noise in spectra. But digital isn't magic. Like analog design, digital design has to be done right!

Digital filters improve signal-to-noise by reducing the amount of noise that "folds in" to the spectrum and by decreasing digitization noise. But some digital filters result in degraded baselines and produce FIDs with a "build-up curve" that you can't use with all processing software. Varian's Time-Corrected Zero-Phase Digital Filters™ give you S/N improvement, flat baselines, and "normal" FIDs — all at the same time.

When dynamic range becomes a problem and you need to reduce the gain on your spectrometer, signal-to-noise can degrade substantially. Varian's Real-time DSP, with its high sampling rate and 20-bit precision, lets you obtain full S/N at lower gains and optimum S/N at any gain.

At Varian, we sell performance, not buzzwords. To arrange a demonstration of Varian's superior DSP capabilities, contact the Varian office nearest you.
DSP from Varian—Designed for Superior Performance

![Graph](https://via.placeholder.com/150)

Plot of S/N vs receiver gain with and without DSP, showing the large improvements possible with Varian’s DSP.

3D NOESY of 10mM lysosyme using DSP with absolutely no baseline correction or linear prediction. The expanded stacked plot on the right shows some of the weaker cross-peaks with no hint of “wandering baseline”.

### Feature

- Real-time digital filters (available on UNITYNOVA™ and UNITYplus™)
  - Time-Corrected Zero-Phase Digital Filters™
  - Choice of real-time digital filters
  - AnalogPlus™ filter
  - Brickwall filter
  - 400 kHz sampling rate (UNITYNOVA only)
  - 20-bit precision
  - No “build-up curve” at front of FID
- Inline digital filters, processing data after acquisition but before storage on host computer (available on all Sun-based Varian spectrometers including UNITYNOVA and GEMINI 2000)
- Post-acquisition digital filtering (available on all Sun-based Varian spectrometers including UNITYNOVA and GEMINI 2000)
  - User-programmable coefficients
  - Frequency shifting
- Low receiver noise floor

### Benefit

- Minimize data storage requirements in acquisition and host computers
- Superior baseline performance
- Optimize performance based on application
- Improves S/N up to 10% without sacrificing baseline performance
- Quantitative accuracy across the entire spectrum
- Greater oversampling brings greater S/N gains
- Obtain the full benefit of oversampling
- FIDs can be processed normally using any software
- Allows full flexibility of digital filtering without the time constraints of real-time filtering; minimizes data storage requirements on host computer
- Allows repeated digital filtering on the same data to allow optimization of parameters
- Any desired digital filter can be used
- Provides bandpass as well as lowpass filters
- Allows DSP to reduce digitization noise and increase S/N
On our Varian^{sup}Inova 500 spectrometer we recently changed the cabling between the probe and the magnet leg. Much to our surprise we suddenly experienced changes in our pulse lengths which were quickly traced to a mistuning of our probe. In particular, the $^{15}N$ coil of our HCN PFG-probe seemed to be affected, since during execution of the pulse sequence the amplifier shut down. This was the result of too much reflected power from the probe. Upon checking the tuning using a wobbler, it was clear that the probe was seriously mismatched, in spite of the fact that we had tuned and matched it using the tune bridge in the magnet leg, and minimized the reading.

Measurement of the "directional coupler" (Mini Circuits ZFSC-2-2, a splitter combiner used in the tune circuit) showed a directivity of only 20.7 dB at 50.6 MHz, clearly insufficient. The values for $^{13}C$ and $^1H$ were not much better (27.5 and 24.9 dB, respectively). As a result, "tuning to zero" on the display does not yield an optimum tune and match. Moreover, the tune and match become strongly dependent upon the electrical length of the circuit. Hence, our sudden change in behavior when changing the cables. This effect becomes even worse if the standard $^{15}N$ filter is used (VSWR = 1.25).

Fortunately, there is a simple solution. Using a minimal amount of hardware, we constructed a device, based upon hybrid ring coupling that provides a directivity of >45 dB (fig. 1). The major components are four pieces of coaxial cable (RG174) with the given electrical lengths. When the probe impedance matches the 50 ohm reference, the "upper" and "lower" RF cancels exactly on the RF-output connector. This device can be used in the normal tune-up setup of our console, i.e. we simply use the console RF and detection circuit. Tune and match now proved to be indistinguishable from the result obtained using a wobbler. The only drawback is the fact that the box is selective for a specific frequency and therefore has to be constructed for every nucleus of interest.

Please credit this contribution to the account of Arno Kentgens.
The compounds shown above are a few examples of custom synthesis compounds that Isotec offers.

Rely on the Leader in Stable Isotopes for Custom Synthesis

Isotec offers the most Flexible Custom Synthesis available!

Since 1987, Isotec has been engaged in the custom synthesis of compounds labelled with stable isotopes. Our synthesis team is composed of experienced professionals and led by an impressive group of Ph.D. chemists. We’ve brought these experts together from such reputable institutions as Merck and Los Alamos National Labs stable isotopes programs to form an exceptional team at Isotec.

The Isotec Advantage
Isotec does not depend on any outside sources to supply our starting material. Today, Isotec is the only commercial producer that separates and enriches over 30 different stable isotopes, including $^{13}$C, $^{17}$O, $^{18}$O, $^{15}$N and Deuterium. This independence gives us a tremendous cost savings and delivery time advantage in custom synthesis. Our on-site production capabilities and ready supply of basic starting material give Isotec a head start in providing rapid custom synthesis of new compounds.

Stable Isotope Solutions
We routinely engage in the multiple step synthesis of isotopically labelled molecules, including metabolites, steroids and standards for environmental, drug, clinical and pharmaceutical applications. We will synthesize quantities ranging from milligrams to kilograms, and also can provide packaging services.

A Reputation of Excellence
We prepare custom synthesis compounds of only the highest purity and superior quality. Our custom synthesis experts are ready to offer you support for your orders and inquiries. Please contact us with your specific requests. Client confidentiality can be guaranteed.

For more information, technical assistance, or to place an order, please call us toll-free at 1-800-448-9760.

ISOTEC INC.
3858 Benner Road
Miamisburg, OH 45342 U.S.A.
(937) 859-1808
Fax (937) 859-4878
isosales@isotec.com
http://www.isotec.com

Isotec, A Matheson, USA Company
Promoting Research and Discovery
The above Amino Acids are a representative sample of double labelled compounds currently available from Isotec. Our chemists regularly synthesize a variety of Carbon-13, Nitrogen-15 double-labelled compounds as well as many other isotopically labelled compounds.

Rely on the Leader in Stable Isotopes for Solid State NMR Products

Isotopically Labelled Compounds for REDOR & other NMR Applications

Isotec supports REDOR applications through the synthesis of consistently high quality double labelled compounds. As the world's largest commercial producer of stable isotopes, our labs are well equipped to fulfill all of your custom synthesis needs.

Custom Synthesis Experts
Our chemists have a wide range of experience and regularly produce custom synthesized compounds, giving Isotec a unique inventory. When we commit to synthesis of a compound you can be confident we will deliver as requested. We test our compounds for isotopic enrichment and chemical purity, consistently providing the highest quality products researchers can rely on.

Stable Isotope Solutions
Researchers benefit from higher sensitivity for REDOR applications when using Carbon-13, Nitrogen-15 labels. For wideline experiments, Isotec makes compounds labelled with Deuterium, and your DOR experiments benefit from Oxygen-17 labels. We are proud to provide only the finest products to meet the specific needs of researchers.

No Compromises on Quality
We won't compromise on Quality Control, because we know product integrity is the key to our success - and to yours. Use Isotec labelled compounds for your solid state NMR applications. You'll find consistent, reliable products backed by knowledgeable technical support.

For Information on Custom Synthesis, other Technical Assistance, or to place an order, call 1-800-448-9760.
Ask us about volume discounts.

ISOTEC INC.
3858 Benner Road
Miamisburg, OH 45342 U.S.A.
(937) 859-1808
Fax (937) 859-4878
isosales@isotec.com
http://www.isotec.com

ISOTEC INC.
A Matheson, USA Company
PROMOTING RESEARCH AND DISCOVERY
Dear Dr. Shapiro,

Some time ago we needed the solid-state $^{13}$C NMR spectrum of a cationic sandwich compound just for referencing purposes. Decamethylcobaltocenium hexafluorophosphate, $(C_5Me_5)_2CoPF_6$, seemed to be the compound of choice because of its high symmetry. However, the result was only simple for the methyl groups (signal B in the figure), while the five-membered ring carbons gave a feature near 95 ppm (cf. A in the figure) that contained more information than we were looking for.

The crystal structure revealed that we did not have magnetically different cations in the unit cell, and a spectrum at higher field confirmed that the apparent signal splitting was due to the dipolar interaction of the $I = 7/2$ and 100%-abundant nucleus $^{59}$Co and $^{13}$C.

There are now many papers which illustrate the effect of quadrupolar nuclei on the spectrum of $I = 1/2$ nuclei, and the topic has been reviewed (Harris, R. K.; Olivieri, A. C. Progr. NMR Spectrosc. 1992, 24, 435). But we are not aware of a clear-cut example of the pair $^{59}$Co, $^{13}$C.

From perturbation theory you would expect eight transitions. However, the analysis of part A of the spectrum by drawing corresponding stick patterns was not successful, because some of the experimentally found transitions virtually merge and the intensities of the pattern components are strange. Meanwhile Eric Brouwer of Robin Harris' lab at Durham has performed a more sophisticated simulation, and the whole story will be published soon.

Thank you for the pink reminder and best regards.

Sincerely yours,

(Frank H. Köhler) (Henrike Heise)
WILMAD = NMR

Each Tube Individually Tested

- Over 40 Years #1 in NMR Tube Manufacturing
- All Tubes Made from Pyrex® or Equivalent Glass
- Complete Line of Accessories
- Custom Glass Manufacturing
- Greater than 99% On-Time Delivery

Call today with your order:
800-220-5171
or visit us online:
www.wilmad.com

established 1951
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.

We provide you with the greatest reproducibility and reliability of any tube on the market. No other manufacturer can claim such high quality standards. Just ask a colleague who has been using Wilmad tubes. Our precision tubes are machined inside and out and checked individually to meet exacting specifications for camber and concentricity. We even check for glass stress, so that under pressure or vacuum, your tube will perform. 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>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</td>
<td>32.50</td>
</tr>
<tr>
<td>5 mm</td>
<td>542-PP-8</td>
<td>800</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00010&quot;</td>
<td>0.00015&quot;</td>
<td>37.50</td>
<td>+100</td>
<td>35.00</td>
</tr>
<tr>
<td>5 mm</td>
<td>541-PP-7</td>
<td>800</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00015&quot;</td>
<td>0.00015&quot;</td>
<td>25.50</td>
<td>+100</td>
<td>23.85</td>
</tr>
<tr>
<td>5 mm</td>
<td>541-PP-8</td>
<td>800</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00015&quot;</td>
<td>0.00015&quot;</td>
<td>27.50</td>
<td>+100</td>
<td>25.85</td>
</tr>
<tr>
<td>5 mm</td>
<td>535-PP-7</td>
<td>500</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00005&quot;</td>
<td>0.000025&quot;</td>
<td>15.15</td>
<td>+100</td>
<td>12.85</td>
</tr>
<tr>
<td>5 mm</td>
<td>535-PP-8</td>
<td>500</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00005&quot;</td>
<td>0.000025&quot;</td>
<td>16.65</td>
<td>+100</td>
<td>14.15</td>
</tr>
<tr>
<td>5 mm</td>
<td>528-PP-7</td>
<td>400</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00010&quot;</td>
<td>0.00005&quot;</td>
<td>10.50</td>
<td>+100</td>
<td>9.25</td>
</tr>
<tr>
<td>5 mm</td>
<td>528-PP-8</td>
<td>400</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00010&quot;</td>
<td>0.00005&quot;</td>
<td>11.95</td>
<td>+100</td>
<td>10.15</td>
</tr>
<tr>
<td>5 mm</td>
<td>507-PP-7</td>
<td>360</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00020&quot;</td>
<td>0.00010&quot;</td>
<td>6.95</td>
<td>+100</td>
<td>5.90</td>
</tr>
<tr>
<td>5 mm</td>
<td>507-PP-8</td>
<td>360</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00020&quot;</td>
<td>0.00010&quot;</td>
<td>7.75</td>
<td>+100</td>
<td>6.60</td>
</tr>
<tr>
<td>5 mm</td>
<td>506-PP-7</td>
<td>100</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00020&quot;</td>
<td>0.00020&quot;</td>
<td>5.40</td>
<td>+100</td>
<td>4.80</td>
</tr>
<tr>
<td>5 mm</td>
<td>506-PP-8</td>
<td>100</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00020&quot;</td>
<td>0.00020&quot;</td>
<td>6.45</td>
<td>+100</td>
<td>5.45</td>
</tr>
<tr>
<td>5 mm</td>
<td>506-IM-7</td>
<td>100</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>0.00020&quot;</td>
<td>0.00020&quot;</td>
<td>3.85</td>
<td>+100</td>
<td>3.45</td>
</tr>
<tr>
<td>5 mm</td>
<td>506-IM-8</td>
<td>100</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>0.00020&quot;</td>
<td>0.00020&quot;</td>
<td>4.05</td>
<td>+100</td>
<td>3.65</td>
</tr>
<tr>
<td>5 mm</td>
<td>WG-5MM-THRIFT-7*</td>
<td>60</td>
<td>7 in</td>
<td>0.015&quot;</td>
<td>nominal</td>
<td>nominal</td>
<td>1.49</td>
<td>+100</td>
<td>1.30</td>
</tr>
<tr>
<td>5 mm</td>
<td>WG-5MM-THRIFT-8*</td>
<td>60</td>
<td>8 in</td>
<td>0.015&quot;</td>
<td>nominal</td>
<td>nominal</td>
<td>1.70</td>
<td>+100</td>
<td>1.50</td>
</tr>
</tbody>
</table>

### J. Young Valve 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>541-JY-7</td>
<td>800</td>
<td>7&quot;</td>
<td>0.015&quot;</td>
<td>0.00015&quot;</td>
<td>0.00015&quot;</td>
<td>89.85</td>
<td>+10</td>
<td>81.90</td>
</tr>
<tr>
<td>5 mm</td>
<td>541-JY-8</td>
<td>800</td>
<td>8&quot;</td>
<td>0.015&quot;</td>
<td>0.00015&quot;</td>
<td>0.00015&quot;</td>
<td>89.85</td>
<td>+10</td>
<td>81.90</td>
</tr>
<tr>
<td>5 mm</td>
<td>535-JY-7</td>
<td>500</td>
<td>7&quot;</td>
<td>0.015&quot;</td>
<td>0.00005&quot;</td>
<td>0.000025&quot;</td>
<td>79.85</td>
<td>+10</td>
<td>71.90</td>
</tr>
<tr>
<td>5 mm</td>
<td>535-JY-8</td>
<td>500</td>
<td>8&quot;</td>
<td>0.015&quot;</td>
<td>0.00005&quot;</td>
<td>0.000025&quot;</td>
<td>79.85</td>
<td>+10</td>
<td>71.90</td>
</tr>
<tr>
<td>5 mm</td>
<td>528-JY-7</td>
<td>400</td>
<td>7&quot;</td>
<td>0.015&quot;</td>
<td>0.00010&quot;</td>
<td>0.00005&quot;</td>
<td>75.70</td>
<td>+10</td>
<td>68.10</td>
</tr>
<tr>
<td>5 mm</td>
<td>528-JY-8</td>
<td>400</td>
<td>8&quot;</td>
<td>0.015&quot;</td>
<td>0.00010&quot;</td>
<td>0.00005&quot;</td>
<td>75.70</td>
<td>+10</td>
<td>68.10</td>
</tr>
</tbody>
</table>

### Bruker Microprobe Tube

<table>
<thead>
<tr>
<th>Product Number</th>
<th>Concentricity</th>
<th>Camber</th>
<th>Capillary Volume</th>
<th>Stem ID</th>
<th>Stem OD</th>
<th>Each</th>
<th>Bulk 10+ Each</th>
</tr>
</thead>
<tbody>
<tr>
<td>520-1A</td>
<td>0.00010&quot;</td>
<td>0.0005&quot;</td>
<td>185 µl</td>
<td>2.16 mm</td>
<td>2.50 mm</td>
<td>30.40</td>
<td>27.35</td>
</tr>
</tbody>
</table>

---

*Pyrex® is a registered trademark of Corning Incorporated, Corning, NY.*
Pulsed NMR Sample Tubes

Absolute pulsed NMR experiments (i.e., signal intensity proportional to sample weight) require clean introduction of the sample into the active volume of the probe. This is a simple operation for normal solutions in the large diameter (18mm) absolute probe on the Bruker NMS 120 spectrometer. However, many of our samples have high viscosities (100's of centipoises) and cannot be transferred with Pasteur pipettes. Moreover, the small diameter 10mm probe must be used for variable temperature experiments (including room temperature) or when short deadtimes are required.

Frank Bosco from New Era has worked with our laboratory to design a specialty tube for pulsed NMR experiments on viscous samples (figure 1). The tube incorporates two key design features. The body was shortened to allow introduction of the sample into the bottom of the tube using standard length syringe needles. This is essential for absolute NMR experiments in a 10mm VT probe that has a small active coil volume (~10mm height). The neck of the tube was made from standard wall tubing with a precision i.d. Because the wall thickness is substantial, tube breakage is avoided when inserting the fluted plug. The precision bore ensures a secure seal to preserve sample integrity over an extended period of time. The plug was made in our machine shop from 10mm o.d. PTFE round stock that matched the standard tube diameter to provide smooth insertion and removal over the microswitch that the instrument uses to trigger the acquisition.

Mark Sullivan
Msullivan@herc.com
PS: Please credit this contribution to Tom Neiss' subscription.
Dynamics, Structure and Function of Biological Macromolecules
4th Course of the International School of Structural Biology and Magnetic Resonance
a NATO Advanced Study Institute

Location: Ettore Majorana Centre for Scientific Culture, Erice, Italy
Dates: May 25-June 5, 1999 Number of working days: 10 days

Objective: To summarize the current state of the field of protein studies focusing on the type of information that can be obtained about dynamic processes in proteins by NMR and other physical methods and the implications for protein and drug design.

Fee: $1,200 includes Board and Lodging to be arranged by the Centre. Some financial aid available and any request for aid should be indicated in the application.

Directors:
Oleg Jardetzky, Professor, Department of Molecular Pharmacology, Stanford University School of Medicine, Stanford, CA 94305-5337, USA.
Jean-François Lefèvre, Professor, ESBS, Louis Pasteur University, Bld. Sébastien Brant, 67400 Strasbourg-Illkirch, France.

Apply to Course Registrar: Ms. Robin Holbrook - same address as that for Prof. Jardetzky.
Tel: (1) 650/723-6270, Email: reh@stanford.edu

Lecturers
Cheryl H. Arrowsmith (Ontario Cancer Institute, Toronto, Canada) • Ivano Bertini (Università degli Studi di Firenze, Italy) • Richard R. Ernst (ETH Zentrum, Zürich, Switzerland) • Hans Frauenfelder (Los Alamos National Laboratories, USA) • Cornelius W. Hilbers (University of Nijmegen, The Netherlands) • Oleg Jardetzky (Stanford University, USA) • Jean-François Lefèvre (Université Louis Pasteur, France) • Michael Levitt (Stanford University, USA) • William N. Lipscomb (Harvard University, USA) • Dino Moras (Université Louis Pasteur, France) • Joseph D. Puglisi (Stanford University, USA) • Paul Rösch (Universität Bayreuth, Germany) • Brian D. Sykes (University of Alberta, Edmonton, Canada)
• Wilfred van Gunsteren (ETH Zentrum, Zürich, Switzerland)

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

Voltronics non-magnetic trimmer capacitors:

Every NMR and MRI Test Depends on One Moveable Part!

Features
- They're truly non-magnetic, with magnetic field distortion less than 1 part per 600 million.
- Lifetime is far greater and RF power handling capability higher thanks to our non-rotating piston design.
- Tuning is linear - no reversals.
- Positive stops at minimum and maximum capacitance.
- Extended shafts can be specified because the tuning screw does not move in or out.

Specifications

<table>
<thead>
<tr>
<th>Feature</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency range</td>
<td>to 1.5 GHz</td>
</tr>
<tr>
<td>Working Voltage</td>
<td>to 20 kV</td>
</tr>
<tr>
<td>Capacitance ranges</td>
<td>0.45 pf min. to 120 pf max.</td>
</tr>
<tr>
<td>Sizes</td>
<td>From 0.12 in. to 1 in. dia.</td>
</tr>
<tr>
<td>Mounting styles</td>
<td>All common types</td>
</tr>
<tr>
<td>Magnetic field distortion</td>
<td>&lt;1 part per 600 million</td>
</tr>
</tbody>
</table>

Custom is Standard at Voltronics

Every NMR and MRI system has unique requirements, and we address them all. In fact we built our entire line of non-magnetic trimmers based on specific requests from our customers. We'll gladly modify an existing trimmer design or create a new one to meet the exact needs of your system.

So if you're building NMR or MRI systems, you should be talking to Voltronics. For 25 years, we've delivered the best-performing, most reliable non-magnetic trimmer capacitors available.

Call (973) 586-8585 and discuss your needs with one of our applications engineers.
ISOTEC, Inc., already the world’s leading commercial producer of stable isotopes, is completing the installation of a fifth carbon-13 column to increase its total production of carbon-13 to over 100 kilograms of isotope per year. Isotec’s engineers are building the new carbon-13 isotope separation plant with production to begin in January 1999. This carbon-13 expansion supports the recent increase in demand for carbon-13 labelled breath test substrates, specifically 13C-urea, which is used in breath test for the detection of H. pylori, the bacteria recently linked to ulcers and stomach cancer. Isotec also recently expanded reactor production capacity for 13C-urea in order to meet the market demand. Isotec was the first company to meet the US FDA manufacturing requirements for production of 13C-urea as a bulk drug in support of new drug applications for the urea breath test.

ISOTEC has also started construction of additional oxygen-18 capacity to greatly increase its total production of oxygen-18 isotope. Isotec expects the expansion to increase output beginning in mid 1999 and again substantially in 2000 and 2001 to meet worldwide demand. This oxygen-18 expansion supports the recent increase in demand for Water-18O, used both for metabolic research and radioisotope production.

In addition, to further increase production capacity, the Isotec plant complex has been facilitated to rapidly accept capacity expansion in both carbon-13 and oxygen-18 in coming years. In order to maintain Isotec’s global leadership, and achieve continued low cost economics, Isotec is committed in expanding our technology development in these areas.

Isotec leads the way in moving stable isotopes beyond the research laboratory into commercial applications, including practical and beneficial uses such as diagnosis of disease.

##

Contact: Dr. Tim Saarinen, Ph.D., x 209
MR is offering for sale a Bruker AVANCE 600, currently available due to an unexpected change in laboratory personnel. In addition, we have been offered a fantastic opportunity to provide a brand new Oxford 600 MHz magnet at an unbelievable price. As a result, we are able to offer you this highly valuable system at about one half of list price. This spectrometer represents an ideal opportunity to bring world-class research NMR capability into your laboratory at an unbelievable price. Don't let this very special opportunity pass you by! Contact Arnold or Doug now at 800-443-5486, send us an email at arnold@mrr.com or doug@mrr.com

AVANCE-600 FEATURES:

- **NEW** Oxford 600 magnet
- BOSS-2 28-gradient shim system
- Three RF channels (expandable to eight identical channels)
- GRASP-III triple axis gradients
- 5mm triple inverse, triple gradient probe, $^1$H observe with $^{13}$C/$^{15}$N decoupling and XYZ PFG gradients
- SGI host computer
- Available as a console upgrade or complete system
Due to a special purchase, we are able to offer this fully loaded AMX-500, including an Oxford 500/52 magnet, at an unbelievably low price. The system is configured as an ideal tool for high field, biological NMR research, with many special features (see the list opposite).

Don't let this very special opportunity pass you by! Contact Arnold or Doug now at 800-443-5486, fax us at 978-630-2509 or send us an email at doug@mrr.com or arnold@mrr.com. Also, be sure to check out our web site at www.mrr.com and find out about the many other special offers currently available from MR for NMR systems, parts, upgrades, probes, and services.

Features included with the AMX-500

UNIX-based SGI Indy host computer
Single axis PFG gradients
Three RF channels
PFG Z-Gradient, triple resonance, inverse TXI probe, ¹H observe with ¹³C and ¹⁵N decouple and ²H lock
BCU-05 near-ambient temperature ultra-stabilizer
Oxford cryomagnet
**NEW PRODUCTS**

**CELL GROWTH MEDIA**

<table>
<thead>
<tr>
<th>Product</th>
<th>Description</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>CGM-1000-DPL</td>
<td>Bio-Express Depleted ($^{12}\text{C}, 99.95%; ^{15}\text{N}, 99.97%)$</td>
<td>$750</td>
</tr>
</tbody>
</table>

**BUFFERS AND DETERGENTS**

<table>
<thead>
<tr>
<th>Product</th>
<th>Description</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>DLM-4533</td>
<td>DL-alpha-Phosphatidylcholine, Dimyristoyl ($D_{14}, 98%$) (DMPC)</td>
<td>$800</td>
</tr>
<tr>
<td>DLM-4528</td>
<td>Bis-Tris ($D_{14}, 98%$)</td>
<td>$800</td>
</tr>
<tr>
<td>DLM-4363</td>
<td>2-(N-Morpholino)ethanesulfonic Acid ($D_{13}, 98%$) (MES)</td>
<td>$800</td>
</tr>
<tr>
<td>DLM-4341</td>
<td>DL-alpha-Phosphatidylcholine, Dihexanyloyl ($D_{16}, 98%$) (DHPC)</td>
<td>$800</td>
</tr>
</tbody>
</table>

**NEW LOWER PRICES**

**BIO-EXPRESS® CELL GROWTH MEDIA**

<table>
<thead>
<tr>
<th>Product</th>
<th>Description</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>CGM-3000-CN</td>
<td>Bio-Express-Min ($U-^{13}\text{C}, 97-98%; U-^{15}\text{N}, 96-99%)</td>
<td>$600</td>
</tr>
<tr>
<td>CGM-1000-U</td>
<td>Bio-Express-1000 (unlabeled)</td>
<td>$187</td>
</tr>
<tr>
<td>CGM-1000-C</td>
<td>Bio-Express-1000 ($U-^{13}\text{C}, 97-98%)</td>
<td>$1870</td>
</tr>
<tr>
<td>CGM-1000-D</td>
<td>Bio-Express-1000 ($U-^{15}\text{N}, 96-99%$)</td>
<td>$1237</td>
</tr>
<tr>
<td>CGM-1000-N</td>
<td>Bio-Express-1000 ($U-^{13}\text{C}, 97-98%; U-^{15}\text{N}, 96-99%$)</td>
<td>$800</td>
</tr>
<tr>
<td>CGM-1000-CN</td>
<td>Bio-Express-1000 ($U-^{13}\text{C}, 97-98%; U-^{15}\text{N}, 96-99%$)</td>
<td>$2475</td>
</tr>
<tr>
<td>CGM-1000-CDN-80</td>
<td>Bio-Express-1000 ($U-^{13}\text{C}, 97-98%; U-^{15}\text{N}, 96-99%$; U-D, 80%)</td>
<td>$9562</td>
</tr>
<tr>
<td>CGM-1000-CDN</td>
<td>Bio-Express-1000 ($U-^{13}\text{C}, 97-98%; U-^{15}\text{N}, 96-99%; U-D, 98%)</td>
<td>$9562</td>
</tr>
</tbody>
</table>

**UNIFORMLY LABELED AMINO ACIDS**

<table>
<thead>
<tr>
<th>Product</th>
<th>Description</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>CLM-4320</td>
<td>L-Cysteine ($U-^{13}\text{C}, 98%$)</td>
<td>$800</td>
</tr>
<tr>
<td>CNLM-3871</td>
<td>L-Cysteine ($U-^{13}\text{C}, 98%$; $^{15}\text{N}, 95-99%$)</td>
<td>$875</td>
</tr>
<tr>
<td>CLM-1574</td>
<td>L-Serine ($U-^{13}\text{C}, 97-98%$)</td>
<td>$665</td>
</tr>
<tr>
<td>CNLM-474</td>
<td>L-Serine ($U-^{13}\text{C}, 98%$; $^{15}\text{N}, 95-99%$)</td>
<td>$700</td>
</tr>
</tbody>
</table>

*More New Products on reverse side*
### Uniformly Labeled $^{13}$C, $^{15}$N F-MOC Protected Amino Acids

<table>
<thead>
<tr>
<th>Product Code</th>
<th>Amino Acid</th>
<th>$^{13}$C Label</th>
<th>$^{15}$N Label</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNLM-4355</td>
<td>L-Alanine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 350.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 700.00</td>
</tr>
<tr>
<td>CNLM-4354</td>
<td>L-Asparagine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>Request Price</td>
</tr>
<tr>
<td>CNLM-4356</td>
<td>L-Glutamine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>Request Price</td>
</tr>
<tr>
<td>CNLM-4357</td>
<td>Glycine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 700.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 250.00</td>
</tr>
<tr>
<td>CNLM-4346</td>
<td>L-Isoleucine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 450.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 900.00</td>
</tr>
<tr>
<td>CNLM-4345</td>
<td>L-Leucine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 450.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 900.00</td>
</tr>
<tr>
<td>CNLM-4358</td>
<td>L-Methionine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>Request Price</td>
</tr>
<tr>
<td>CNLM-4362</td>
<td>L-Phenylalanine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 450.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 900.00</td>
</tr>
<tr>
<td>CNLM-4347</td>
<td>L-Proline-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 450.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 900.00</td>
</tr>
<tr>
<td>CNLM-4349</td>
<td>L-Tyrosine-N-FMOC, O-t-ButyI Ether</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 990.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 1900.00</td>
</tr>
<tr>
<td>CNLM-4348</td>
<td>L-Valine-N-FMOC</td>
<td>$^{13}$C, 98%+</td>
<td>$^{15}$N, 96-99%</td>
<td>$0.1 g$ 450.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$0.25 g$ 800.00</td>
</tr>
</tbody>
</table>

### Modified Nucleics

<table>
<thead>
<tr>
<th>Product Code</th>
<th>Nucleic Acid</th>
<th>$^{13}$C Label</th>
<th>$^{15}$N Label</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>DLM-4391</td>
<td>5,6-Dihydrothymine (5, 6-D, methyl-D), 95%+</td>
<td></td>
<td></td>
<td>50 mg 780.00</td>
</tr>
<tr>
<td>CNLM-4392</td>
<td>5-Hydroxycytosine (2-$^{13}$C, 99%; 1,3-$^{15}$N), 98%</td>
<td></td>
<td></td>
<td>25 mg 950.00</td>
</tr>
<tr>
<td>CNLM-4393</td>
<td>5-Hydroxymethyl (4-$^{13}$C, 99%; $^{15}$N), 98%</td>
<td></td>
<td></td>
<td>50 mg 1575.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5 mg 895.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>10 mg 1495.00</td>
</tr>
</tbody>
</table>

### Additional Products

<table>
<thead>
<tr>
<th>Product Code</th>
<th>Product</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>ULM-4482</td>
<td>6-Fluoro-L-Tryptophan (unlabeled)</td>
<td>Request Price</td>
</tr>
<tr>
<td>DLM-4481</td>
<td>6-Fluoro-L-Tryptophan (ring-D), 96-98%</td>
<td>Request Price</td>
</tr>
</tbody>
</table>
Postdoctoral Positions at Argonne

I will have two openings at the postdoctoral level in my laboratory in the Chemistry Division beginning October 1, 1998. The positions will involve research in NMR. Specific projects include developing new solid-state methods for chemical-shift MRI of materials, PFG spin-diffusion of gaseous probes in porous systems, MRI of solvent ingress into heterogeneous polymeric materials, and dipolar recoupling measurements to study self-associating peptides.

The successful candidate should have a recent Ph.D. (within three years) in Chemistry, or closely related field, with some experience in hardware and software development, and with experience in solid-state NMR or MRI and their application to structure elucidation.

The Chemistry Division has state-of-the-art NMR facilities, including two new fully equipped Bruker DMX 500 and Bruker DSX-200/100 systems with a full complement of solids, liquids and imaging capabilities, a home-built Tecmag 400 imaging/spectroscopy system, a GE Omega 300, and Varian INOVA 300 spectrometer, and several IBM R-6000 and Silicon Graphics workstations for advanced data processing, calculation and data refinement.

For further information contact:

Robert E. Botto
Chemistry Division
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, IL 60439
Ph: (708)252-3524  FAX: (708)252-9288
e-mail: robert_botto@gmgate.anl.gov

POSTDOCTORAL POSITION – NMR SPECTROSCOPY

Sandia National Laboratories (SNL), operated by Lockheed Martin for the Department of Energy, located in Albuquerque, NM has an immediate opening for a postdoctoral position in solid state NMR spectroscopy. The position will involve NMR investigations and characterization of a variety of materials including glasses, ceramics, polymers and hybrid materials. A major portion of the research will include the implementation of heteronuclear and multinuclear solid state NMR experiments to probe the chemistry and medium range structural order in oxide glasses, but a variety of other materials collaborations are possible. A Ph.D. in chemistry, physics, material chemistry or related field is required. Demonstrated competence in advanced solid state NMR techniques, computational methods and material preparation are preferred. The research will be carried out in close collaboration with SNL research staff members, but the applicant is expected to have demonstrated the ability to perform independent research, along with excellent communication skills. This position will be for one year, and is renewable for up to three years. The program is open to all qualified U.S. citizens without regard to race, color, age, religion, sex, or national origin. Interested candidates should send a resume and the names of three references to: Dr. Todd M. Alam (tmalam@sandia.gov), Sandia National Laboratories, MS 1407, Org. 1811, Albuquerque, NM 87185-1407.
Another Blast from the Past

A quotation from the baroque era of NMR - note the date!

"Nuclear and Electron Spin Magnetic Resonance"

by

John E. Wertz

(Chem. Rev. 55, 829-953 (1955)

III. CHEMICAL SHIELDING

"At a time when physicists were busy comparing magnetogyric ratios of various nuclei and expressing these to seven or more significant figures, several disquieting papers appeared (147, 312, 443). It was reported that in compounds of phosphorus, nitrogen, and fluorine the resonant frequency for a particular nucleus depended on the compound in which it was present. This effect was called the "chemical shift," because physicists could think of no stronger term of damnation for an effect which was making insignificant several digits in their nuclear moment data."
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. 483 (Dec.) 27 Nov. 1998
No. 484 (Jan.) 24 Dec. 1998
No. 485 (Feb.) 22 Jan. 1999
No. 486 (Mar.) 19 Feb. 1999
No. 487 (Apr.) 23 May 1999

* 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

The Newsletter's fiscal viability depends very heavily on the funds provided by our Advertisers and Sponsors. Please do whatever you can to let them know that their support is noted and appreciated.

Mailing Label Adornment: Is Your Dot Red?

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

Forthcoming NMR Meetings, continued from page 1:

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; (415) 723-6270; Fax: (415) 723-2253; Email: reh@stanford.edu. See Newsletter 482, 28.

Additional listings of meetings, etc., are invited.
How To Run JEOL's Eclipse+ Spectrometer

Step 1: Enter your sample name and the solvent.
Step 2: Click the mouse button on the data you want.
Step 3: Walk away with your data.

JEOL's Eclipse Spectrometer will automatically do everything else for you.

- Auto Probe Tuning (with AutoTune Broad Band Probe)
- Auto-sample Control (with AutoSample Changer)
- Auto Selection of Spectrometer Conditions
- Auto Baseline Correction
- Auto Data Presentation
- Auto Phase Correction
- Auto Digital Filtering
- Auto S/N Monitoring
- Auto Queue Control
- Auto Receiver Gain
- Auto Data Storage
- Auto Referencing
- Auto Processing
- Auto Peak Picks
- Auto Integration
- Auto Plotting
- Auto Shim
- Auto Lock

JEOL USA, Inc., 11 Dearborn Road, Peabody, MA 01960
Tel: (508)535-5900  Fax: (508)536-2205
Email: nmr@jeol.com  WWW: http://www.jeol.com