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A monthly collection of informal private letters from Laboratories of NMR. Information contained herein is solely for the use of the reader. Quotation is not permitted, except by direct arrangement with the author of the letter, and the material quoted must be referred to as a "Private Communication." Reference to the TAMU NMR Newsletter by name in the open literature is strictly forbidden.

These restrictions apply equally to both the actual Newsletter participant-recipients 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 of exchange of NMR information.
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Write or call for our new Catalog 781.
FT NMR was never "hard," only certain samples were. Now with the low cost JEOL FX60QS System, High Resolution Solid State NMR becomes routine.
Dear Professor Shapiro,

TEMPERATURE AND LSR EFFECTS ON $^1$H SHIFTS IN DIBENZO CYCLOHEPTATRienes

We have referred previously to $^1$H solvent shifts (TAMNMR 217/17) and J errors (TAMNMR 237/19) in dibenz[b,f]oxepin(I) and its nitrogen analogue. Dr. J.A.G. Drake's INDO/CON III analyses of the 220 MHz $^1$H spectra of the related compounds 5H-dibenzo[a,d]cyclohepten-5-one (or dibenzo[b,f]tropone) (II) and 5H-dibenzo[a,d]cyclohepten-5-ol (III) show that the chemical shifts have linear solvent and temperature dependences over the ranges studied (Table). At low concentrations of III in chloroform-d$_1$ solution, two peaks emerge for each of the H(5) and OH(a and b), possibly indicative of the presence of a protonated species (slow decomposition occurs). The predominantly negative $\delta$ (Table) may be due, as suggested for I, to the predominance of (reaction-field) deshielding, arising from changes in dielectric constant of the solvent, over the increased shielding to be expected, as temperature is decreased, from closer association between solute molecules (analogous to the effect of increased concentration). Addition of Eu(fod)$_3$ to II in chloroform-d$_1$ induces $^1$H paramagnetic shifts, H(4)$>$H(11)$>$H(1)$>$H(3)$>$H(2), directly proportional to the metal/substrate ratio over the range studied and consistent both with the $^1$H chemical-shift assignment and with complexing of the reagent metal ion to the carbonyl oxygen in II. H(4) in II is distinctive in having the largest LIS shift ratio and also in having a positive $\delta$ coefficient.

Incidentally, measurements on fluoren-9-one, briefly reported in TAMNMR 256/11, have been extended to 1-methylfluorene and truxene.

Yours sincerely,

D. W. Jones

Table 1H shifts extrapolated to 273 K (δ, ppm) and temperature shifts (θ, 10^3 ppm K^-1) from 220 MHz spectra of (i) II in 0.50 mol dm^-3 CDCl_3 (224-322 K); (ii) II in 0.08 mol dm^-3 CS_2 (247-294 K); and (iii) III in 0.13 mol dm^-3 CDCl_3 (269-320 K).

<table>
<thead>
<tr>
<th>Proton</th>
<th>(i) II in CDCl_3</th>
<th>(ii) II in CS_2</th>
<th>(iii) III in CDCl_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(1)</td>
<td>7.482 -0.38</td>
<td>7.420 -0.12</td>
<td>7.368 -0.66</td>
</tr>
<tr>
<td>H(2)</td>
<td>7.585 -0.59</td>
<td>7.530 -0.26</td>
<td>7.285 -0.69</td>
</tr>
<tr>
<td>H(3)</td>
<td>7.512 -0.57</td>
<td>7.440 -0.18</td>
<td>7.413 -0.62</td>
</tr>
<tr>
<td>H(4)</td>
<td>8.196 0.21</td>
<td>8.060 0.89</td>
<td>7.654 -0.26</td>
</tr>
<tr>
<td>H(5)</td>
<td>- -</td>
<td>- -</td>
<td>5.384 +0.17</td>
</tr>
<tr>
<td>OHa</td>
<td>- -</td>
<td>- -</td>
<td>2.541 -3.21</td>
</tr>
<tr>
<td>b</td>
<td>- -</td>
<td>- -</td>
<td>2.521 -3.18</td>
</tr>
<tr>
<td>H(11)</td>
<td>6.994 -0.34</td>
<td>6.945 -0.14</td>
<td>7.104 -0.53</td>
</tr>
<tr>
<td>CHCl_3</td>
<td>7.245 -0.30</td>
<td>- -</td>
<td>7.246 -0.42</td>
</tr>
</tbody>
</table>

[Diagram of chemical structures]
Dear Professor Shapiro:

We are currently involved in a large project on COLIPASE, a small protein (93 residues) which, as a cofactor of pancreatic lipase, plays a key role in the intraduodenal lipolysis of dietary triglycerides. Besides its biological importance, the lipase/colipase/substrate interface system constitutes an attractive model to study protein-protein and protein-lipid interactions. We have recently identified a particular hydrophobic aromatic domain on colipase as being the Lipid Binding Site (P. Canioni and P. Cozzone, Biochimie 1979, 61, 343-354 and FEBS Lett. 1979, 97, 353-357 – P. Canioni, P. Cozzone and L. Sarda, Biochim. Biophys. Acta 1980, 621, 29-42). Two tyrosine residues located in the segment 50-57 of this domain are involved in the binding process and give a strong photo-CIDNP effect in presence of a lumiflavin dye (P. Canioni, P. Cozzone and R. Kaptein, FEBS Lett. 1980, 11, 219-221). In collaboration with Paul Canioni and Louis Sarda at this laboratory and Robert Kaptein at the University of Groningen we have conducted in Groningen a series of laser photo-CIDNP experiments at 360 MHz on several colipase-micelle complexes to document the influence of charge effects on the association.

In presence of sodium taurodeoxycholate (TDC) micelles, the CIDNP effect on both Tyr residues is totally suppressed at neutral pH (Fig. 1 and 2a). Under these conditions, the 2 aromatic surface residues are no longer accessible to the dye due to the protection by the TDC-micelle. Electrostatic repulsions between phenolate and TDC negative charges at high pH induce the disruption of the complex which is accompanied by a gradual restoration of the polarization of the 2 tyrosines (Fig. 2).

We have subsequently interacted colipase with chenocholamine, a detergent which bears a positive charge up to around pH 11. As expected, the association remains tight even at pH 11.2 as shown by the almost complete absence of CIDNP effect on the tyrosines at all pH values (Fig. 3). In both cases, the emission line of the C(2)-H proton of His I (His 30) remains present in the complex, illustrating the fact that this residue does not belong to the Lipid Binding Site.
We think that this series of straightforward experiments illustrate very well the potentials of the laser photo-CIDNP technique to study binding processes.

Sincerely yours,

Patrick J. Cozzone

Fig. 1

360 MHz proton NMR spectrum and photo-CIDNP difference spectrum of porcine colipase A. Experiments were performed at 35°C in 12 mM TDC with 150 mM NaCl and 0.4 mM flavin at pH 7.65. Concentration of colipase: 1.5 mM (a) dark spectrum, (b) photo-CIDNP difference spectrum. Light and dark FID's were taken alternately (20 scans); (c) photo-CIDNP difference spectrum of colipase in the absence of TDC (pH 7.2).

Fig. 2

TDC

Fig. 3

chenocholamine
Dear Barry,

threatened by your green reminder I am forced to reveal a first glimpse of our new baby, a program for "interpretation of CNMR spectra". In contrast to conventional search programs scanning large data bases for similar or identical reference spectra, this program relies solely on a description of the expectation ranges of chemical shifts in characteristic substructures. On the other hand only large structure linked data collections allow a realistic estimate on the influence of structural changes on spectral features and thereby the prediction of possible substructural units. The enclosed example shows a similarity search (SAHO) and an interpretation for the spectrum of 3'-methylacetophenone. The suggested structural units leave only one solution, namely the correct answer.

That's all for this year. Best regards,

Wolfgang

Enclosure
EINGEGEBENE LINIEN MIT MULTIPLIZ. UND INTENSITÄT:
1. 197.9 PPM  S  1
2. 138.3 PPM  S  1
3. 137.3 PPM  S  1
4. 133.8 PPM  D  1
5. 128.8 PPM  D  1
6. 128.5 PPM  D  1
7. 125.6 PPM  D  1
8. 26.5 PPM   Q  1
9. 21.2 PPM   Q  1

EINGABEOPTION ?(N;K;++;E)
=E

SUCHLAUF STARTEN ?
=J

----------------------------------------
SP E K T R E N - S U C H E
----------------------------------------

MIT 30757 SPEKTREN

ERGEBNIS: 10 SPEKTREN

SPEKTRUM NAME
CNMR5764 4'-METHYL-ACETOPHENONE
CNMR6327 3'-METHYL-ACETOPHENONE
CNMR7344 2'-METHYL-ACETOPHENONE
ZUSÄTZLICH 7 TOECHTER

INTERPRETATION ?
=J

----------------------------------------
SP E K T R E N I N T E R P R E T AT I O N
----------------------------------------

4.168 (13) - ASYM. DISUBST. BENZENE
1.821 (54) - ACETYL (AROM) OHNE ORTHO-SUBST.
1.625 (7)  - METHYL (AROM) OHNE ORTHO-SUBST.

KEINE WEITEREN LINIEN

ANFANGSBUCHSTABEN DES GEWÜNSCHTEN SYSTEMS?
=E
December 1, 1980

Professor B. L. Shapiro
Department of Chemistry
Texas A & M University
College Station
Texas 77843

Dear Professor Shapiro:

I would like to announce the 6th AMPERE Summer School on Biological Applications of NMR to be held September 8-18, 1981, in Schloss Seggau bei Leibnitz, Steiermark, Austria. The school will consist of lectures, group discussions and problem sessions and is intended both for spectrotscopists and for biochemists. Topics to be covered include: Basic principles of NMR spectroscopy; New techniques: 2DFT, relaxation analysis, photo-CIDNP; NMR of macromolecules—methodology for resolution and assignment of signals; Proteins: structure, dynamics and interactions with small molecules; Nucleic acids: structure, dynamics and interactions with small molecules; NMR studies of enzyme mechanisms; Membranes: molecular motion, protein-lipid interactions; NMR of whole cells and organs: 13C and 31P studies of metabolism and metabolic regulation, NMR imaging in vivo.

Following is a tentative list of the faculty: E.R. Andrew (Nottingham), I.D. Campbell (Oxford), P. Cozzone (Marseilles), R.A. Dwek (Oxford), R.R. Ernst (Zurich), K. Hausser (Heidelberg), R. Kaptein (Groningen), M.P. Klein (Berkeley), P.C. Lauterbur (Stony Brook), J.L. Markley (Purdue), E. Oldfield (Urbana), D. Patel (Murray Hill), W.D. Phillips (St. Louis), J.H. Prestegard (Yale), G.K. Radda (Oxford), B.R. Reid (Seattle), J. Seelig (Basel), R.C. Shulman (Yale), I.C.P. Smith (Ottawa), A. Xavier (Lisboa) and members of the Organizing Committee.

Members of the International Organizing Committee are O. Jardetzky (Stanford, USA) Chairman, V. Bystrov (Moscow, USSR), S. Forsen (Lund, Sweden), G.C.K. Roberts (London, UK), K. Wilthrich (Zurich, Switzerland).

Attendance is limited to 120 participants and the cost is 3000 Austrian Schillings, including room and board. Applications should include a brief curriculum vitae and a letter of recommendation from a university faculty member. DEADLINE FOR APPLICATION is April 1, 1981. Applicants will be notified of the decision on their application by May 1, 1981. Letters of application and all correspondence should be addressed to: Dr. G.C.K. Roberts, National Institute for Medical Research, The Ridgeway, Mill Hill, London NW7 1AA, England. Telegrams: Natimmed London NW7. Telephone: 01-959 3666.

Yours sincerely,

Oleg Jardetzky
If you can’t observe solids as readily as liquids on your superconducting FT NMR...

...you just don’t have an XL-200!

With the new 13C solid-state accessory for the XL-200, you can spin solid or powdered samples at the magic angle, increase sensitivity using cross-polarization, and achieve efficient line narrowing with strong dipolar decoupling. Yet operation is surprisingly simple! You can introduce and eject the rotor pneumatically without disturbing the probe or the spinning axis adjustment. You monitor the spin rate on the spectrometer’s built-in tachometer, just as in liquid-sample experiments. Front panel controls let you adjust optimal cross-polarization and decoupling conditions independently and conveniently.

There are other unique aspects to the XL-200 superconducting FT NMR Spectrometer, such as the data handling and spectrometer control system: a 13-bit ADC, which accommodates stronger signals on each transient; a standard 32K CPU, independent of the acquisition processor and programmed in PASCAL, a high-level, structured language, a built-in interactive SM-word disk with dual platters; a large, flicker-free raster scan display.

The software, too, is exceptionally sophisticated. It permits multitasking (simultaneous acquisition, processing, printing, etc.) and queuing (automatic sequential execution of requested tasks) on the same or on different NMR experiments. You can also array parameters (up to three variables, including temperature) within a given experiment; generate your own convenient macro-commands; create your own special or general-purpose pulse sequences in a simple, English-like code; even do your own computer programming in PASCAL.

Then there’s the matter of the XL-200’s broadband accessory which, with only a single probe for liquid samples, enables you to observe a host of nuclei (including 13C) between 20 and 81 MHz. And there’s the remarkable low-loss dewar system, which operates over three months on only 25 liters of liquid helium.

The XL-200 is in a class by itself—
with a price tag and an operating economy that belie its advanced design.

*Sample courtesy of E. I. Du Pont de Nemours and Company*
Title: Molecular order in Liquid Crystals with opposite diamagnetic anisotropies

Dear Prof. Shapiro,

We just received your "dangerous Yellow weapon!" Before it really 'hurts' us, we submit the following contribution.

Recently, we have studied the variation of the orientation of molecules dissolved in liquid crystals with positive and negative diamagnetic anisotropies and in the mixture of the two types of the solvents, in connection with our search for finding out convenient ways and means for changing the molecular order at 'will'. We studied the proton NMR spectra of benzene oriented in the nematic phases of Merck ZLI-1167 and N-(p-ethoxybenzylidene)-p-n-butylamiline (EBBA) and in the mixtures of the two. The PMR experiments were conducted in 3 weight per cent solutions of benzene in ZLI-1167 (solution I) and EBBA (solution II) separately. Then known amounts of solution (II) were gradually added to solution (I) and the spectra were recorded at each concentration. At a critical concentration, we found that the dipolar couplings change to twice their values and have opposite signs. The results can be interpreted in terms of the change of the angle between the directions of the optic axis of the liquid crystal and the applied magnetic field from 90° to 0°. Above the critical concentration, the molecules orient like in solution (II), i.e., with the optic axis along the direction of the magnetic field. Below the critical concentration, the preferred orientation is like that in solution (I). Further studies and possible applications of this observation are in progress.

With regards,

Yours sincerely,

C.L. Khetrapal  A.O. Kunwar

C.L. Khetrapal  A.O. Kunwar
Photodimerisation of 2-chloro-1,4-naphthoquinone can lead to four possible symmetrical dimers (1-4). Dimers (3) and (1) were isolated after sunlight irradiation of an acetic anhydride solution and crystalline 2-chloro-1,4-naphthoquinone, respectively, whereas dimer (4) was synthesized from 1,2-phthaloyl-2a-chloro-2a,3,8,8a-tetrahydro-3,8-dioxonaphtho[b]cyclobutadiene. The structures of these dimers were elucidated from extensive 1H and 13C n.m.r. studies. In determining the configuration of the cyclobutane rings a knowledge of the signs of the (H,H) and (C,H) couplings in these moieties have been especially useful.

The two protons (A and M) and a 13C methine carbon atom (X) of the cyclobutane ring of the dimers formed an AMX spin system. The relative signs of the (H,H) [J(AM)], directly-bonded (C,H) [J(AX)] and over more than one bond (C,H) [J(MX)] coupling constants were determined with 13C-{1H} SPI experiments. The magnitude of the (H,H) coupling constants were obtained from 13C-satellite 1H n.m.r. spectra. The experimental values for the three dimers are given in the Table.

<table>
<thead>
<tr>
<th>TABLE (C,H) and (H,H) coupling constants</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimer:</td>
<td>1</td>
<td>2*</td>
<td>3</td>
</tr>
<tr>
<td>J(CH)*</td>
<td>151.2</td>
<td>148.6</td>
<td>148.6</td>
</tr>
<tr>
<td>J(CH)</td>
<td>-6.3</td>
<td>+</td>
<td>-4.9</td>
</tr>
<tr>
<td>J(HH)</td>
<td>+11.2</td>
<td>+</td>
<td>+4.0</td>
</tr>
</tbody>
</table>

* Assumed positive. † Expected signs

A cross-ring 4J(HH) in cyclobutane is small and positive when the interacting protons are cis and negative when they are trans3. 3J(CH) and 3J(CU) are normally assumed positive, whereas 2J(CH) can be negative or positive*4. 2J(CH) is negative in the cyclobutane moiety of the dimers.
Only the signs of the (H,H) and (C,H) couplings, between the protons and a methine carbon atom of the cyclobutane ring of the dimers, are required to distinguish between dimers (1,3), (2) and (4). One could differentiate between dimers with configurations (1) and (3) from the magnitude of these coupling constants.

Yours sincerely

P.L. Wessels
SENIOR CHIEF RESEARCH OFFICER

Prof. B. L. Shapiro  
Dept. of Chemistry  
Texas A & M University  
College Station  
TX 77843  

December 2, 1980

Dear Prof. Shapiro:

In connection with some of our synthetic projects in carbohydrate chemistry, we achieved the synthesis of the dihydro-4-pyrone II, namely 2,4,6-tri-O-acetyl-1-deoxy-D-erythrohex-1-enopyranos-3-ulose, in only two steps from the commercially available 1,2:5,6-di-O-isopropylidene-3-ketoglucofuranose (I) as shown below:

II had been prepared earlier by much longer routes starting from different precursors and its characterization by proton NMR had been only partial1-3. We present here a complete analysis of the same by proton (at 200 MHz) and C-13 NMR spectroscopy.

1549 Albany Street, Boston, Massachusetts 02118

Telephone 617-482-9595
Telex 94-0996
$^1$H and $^{13}$C nmr spectral parameters for 11b

<table>
<thead>
<tr>
<th>Position</th>
<th>$^1$H shift (ppm)</th>
<th>$^1$H, $^1$H (Hz)</th>
<th>$^{13}$C shift ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-1</td>
<td>7.47s</td>
<td>-</td>
<td>155.38d</td>
</tr>
<tr>
<td>C-2</td>
<td>-</td>
<td>-</td>
<td>130.56s</td>
</tr>
<tr>
<td>C-3</td>
<td>-</td>
<td>-</td>
<td>181.94s</td>
</tr>
<tr>
<td>C-4</td>
<td>5.67d</td>
<td>$J_{4,5}=13.18$</td>
<td>67.77d</td>
</tr>
<tr>
<td>C-5</td>
<td>4.70dt</td>
<td>$J_{5,4}=13.18$</td>
<td>79.04d</td>
</tr>
<tr>
<td></td>
<td>$J_{5,6}=3.78$</td>
<td>$J_{5,6}'=2.57$</td>
<td></td>
</tr>
<tr>
<td>C-6</td>
<td>4.41m</td>
<td>$J_{6,5}=12.82$</td>
<td>61.23t</td>
</tr>
<tr>
<td></td>
<td>$J_{6,5}'=3.78$</td>
<td>$J_{6,5}''=2.57$</td>
<td></td>
</tr>
<tr>
<td>COCH3's</td>
<td>2.13s</td>
<td>-</td>
<td>20.08, 20.35, 20.59q</td>
</tr>
<tr>
<td></td>
<td>2.19s</td>
<td></td>
<td>168.48, 168.96, 170.32s</td>
</tr>
<tr>
<td></td>
<td>2.24s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

a. chemical shifts from internal TMS for CDCl₃ solutions; s=singlet, d=doublet, t=triplet, q=quartet and m=multiplet and apply to the $^1$H resonances; s, d, t and q apply to proton off-resonance decoupled C-13 spectrum.

With best regards,

Lawrence P. Thomas

Sincerely,

Puliyur R. Srinivasan

Surendra Gupta

Douglas Moakley

References:

December 2, 1980

Dear Barry:

The word "universal" has a nice ring to it, and isn't too much of an exaggeration, I trust. In actuality, though, this Field/Frequency lock has so far proved itself on a pulsed NMR machine used to do $T_1$ and $T_2$ measurements of protons from 8 to 60 MHz. For high resolution work one would need to phase lock the Observe and Lock Frequency synthesizers. Other Fields (supercon?), absorption mode display etc. are obvious variations on the theme. In fact the theme itself is pretty obvious, although it may never have been played before with this broad band sound.

This is a time-shared lock system, where the transmitter is on 25% of the time and the receiver about 65% of the time. There is a 10% wait after the transmitter pulse so that the receiver can recover. The repetition rate is 1KHz, although 10KHz or 20KHz might be better to prevent possible spikes in high resolution applications. Transmit and Receive is done centerband for simplicity's sake. The transmitter gating has to be done pretty thoroughly, and the synthesizer has to be reasonably well shielded from the outside world. As gates we used two double balanced mixers (Mini-circuits Lab's SRA-1) in series before the power amplifier, and followed the P.A. by series crossed PIN diodes, all three gates being switched by the timer. No transmitter leakage was measurable. The R.F. power is controlled by the turn-on current to the SRA-1's.

The broadband continuously variable phase shifter involved the use of a varactor and AGC to produce four channels of R.F. with 90° shifts between them and applied to four equally spaced taps on a potentiometer. In retrospect I think it would have been easier to employ a broadband quadrature hybrid (Anzac) for the 90° shifts. The input to either of these phase shifters must be a sine wave. Since our synthesizer (Syntest) delivered a square wave, we had to make a broadband square-to-sine converter (not shown). The ultimate system would probably use a more expensive synthesizer delivering a sine wave and phase coherent with the Observe frequency synthesizer.

We chose lithium as a lock substance partly because of its frequency being compatible with a standard Syntest Synthesizer. The sample was concentrated LiCl doped with MnCl$_2$ to give a broader line.
The transmitter drives the probe via a broadband Transmit/Receive circuit (J.L. Engle, TAMU NMR, June 1979). The probe has a small sample tube close to the Observe sample. Two lock sample coils are used and a two-position range switch. Toning and a reasonable match are accomplished with one variable capacitor (J.L. Engle TAMU NMR Nov. 1976 p.24). Resonance is indicated by a reflectometer permanently installed in the transmitter line. The preamplifier is broadband, and low noise when it sees an approx. 50 ohm source. We used discrete components, with an NEC's NC921 transistor at the input.

The receiver is gated in two places: The reference gate is another SRA-1. The AF amplifier gate is a junction field effect transistor preceding an integrator at the output to the super stabilizer. The mixer is an SRA-1.

The timer clock is a free running multivibrator with a 25% duty cycle as used by the transmitter. A pulse stretcher adds the time used for receiver recovery.

Please credit this to Dr. M. Cohn's account.

Sincerely,

James L. Engle
Prof. B.L. Shapiro  
Texas A. & M. University  
College of Science  
College Station, Texas 77843  
U. S. A.

Title: "Quantitative $^{13}$C nmr of petroleum products"

Dear Prof. Shapiro,

quantitative $^{13}$C nmr has important application in complex samples where other analytical methods fail or are tedious. One favorable case is the characterization of petroleum cuts and coal-derived products. The $^{13}$C nmr spectrum enables the distribution of the different carbon types to be determined with a minimum of structural hypothesis. An important information which can be easily derived is the "aromaticity", that is the fraction of aromatic carbon $\frac{C^A}{C^T}$.

The nmr experiment requires peculiar conditions. The relevant operational parameters which should be optimized in order to obtain the same sensitivity for all carbons and the highest S/N are the flip angle, the acquisition time, the pulse delay (using proton gated decoupling) and the relaxation agent concentration.

A pitfall of the method, however, is that one uses a simple aromatic mixture as standard test. To the best of our knowledge no comparison with an independent analysis on a complex mixture has been done.

By the nmr method we have investigated several atmospheric gasoils, and the corresponding hydrotreated products, at different content of aromatic compounds ranging from 7 to 30%.

...
We have also analyzed these samples by mass spectrometry, according to a well known procedure\(^3\) and we have got an hydrocarbon types distribution\(^4\) which can be translated into the fraction of aromatic carbon. The final results of the two methods are collected in the Table 1 together with the aromatic product percentage determined by liquid-solid chromatography\(^5\). The two series of data are in good agreement, confirming the reliability of both methods.

The figure shows also the good correlation obtained between the aromatic product concentration in the gasoil and the aromaticity.

Yours sincerely,

E. Santoro, G. Bragato

References

2) Kindly provided by Dr. G. Matarrese (Bollate Research Center).
3) ASTM Method n. D2425.
4) Thanks are due to Dr. L. Motta (Bollate Research Center) for the mass spectral data.
5) ASTM Method n. D2549.
Table 1 - Aromaticity ($C_{Ar}/C_{Tot}$) of gasoil by $^{13}$C nmr and mass spectrometry.

<table>
<thead>
<tr>
<th>Sample</th>
<th>% by wt. of arom.comp.</th>
<th>Aromaticity: $C_{Ar}/C_{Tot}$</th>
<th>Experimental $^{13}$C nmr conditions (Bruker WH 90/DS)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>13C nmr</td>
<td>Mass.Spectr.</td>
</tr>
<tr>
<td>1</td>
<td>29.5</td>
<td>0.16</td>
<td>0.17</td>
</tr>
<tr>
<td>2</td>
<td>22.0</td>
<td>0.086</td>
<td>0.108</td>
</tr>
<tr>
<td>3</td>
<td>17.0</td>
<td>0.075</td>
<td>0.088</td>
</tr>
<tr>
<td>4</td>
<td>16.6</td>
<td>0.087</td>
<td>0.087</td>
</tr>
<tr>
<td>5</td>
<td>11.1</td>
<td>0.055</td>
<td>0.058</td>
</tr>
<tr>
<td>6</td>
<td>9.6</td>
<td>0.046</td>
<td>0.047</td>
</tr>
<tr>
<td>7</td>
<td>8.2</td>
<td>0.041</td>
<td>0.043</td>
</tr>
<tr>
<td>8</td>
<td>7.1</td>
<td>0.026</td>
<td>0.035</td>
</tr>
</tbody>
</table>

![Graph](image)

**Fig. 1 - Aromaticity ($C_{Ar}/C_{Tot}$) vs. % aromatic product in the gasoil.**
Never before in the history of NMR has time so optimally been shared between processes. Bruker’s DISNMR, the first true time-sharing NMR data system allows you to process several data sets simultaneously. For example: you may perform more than one Fourier transformation while executing a PASCAL program at the same time.

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Institute/Company: ________________________________

Address: ______________________________________

City/State/Zip: ________________________________
5th European Experimental NMR Conference

Dear Professor Shapiro:

The next (5th) European Experimental NMR Conference will be held at Königstein/Frankfurt (Main), West Germany. Registration will begin Tuesday, May 12, 1981, and the program will run through noon on Friday, May 15. Sessions are planned in the areas of new techniques in liquids, solid state NMR, 2D NMR, NMR imaging, computer aids, metal nuclei NMR and others. Further information and the Second Circular will be mailed on request. The deadline for contributions will be February 28, 1981.

Sincerely yours,
Dear Professor Shapiro,

NMR of Food Additive Polyphosphates

$^{31}$P FTNMR spectroscopy is a convenient technique for observing the interaction of polyphosphate food additives with a food matrix. We have been studying the behaviour of polyphosphate food additives when injected into enzymatically active chicken meat (1,4). However, the NMR resolution obtained from lumps of meat pushed down into the NMR sample tube is much less than that obtained from solution samples. This is due to difficulties in shimming, inhomogeneous distribution of polyphosphate within the sample, as well as pH and meat structure inhomogeneities. In those instances where a higher resolution is required, the system may be simulated by using the food additive in aqueous solution and the meat sample cut to form the antivortex plug. An example of the method applied to the hydrolysis of tetrapolyphosphate in contact with chicken pectoralis major tissue is shown. The presence of tripolyphosphate signals shows that at least some of the tetrapolyphosphate is hydrolysed via the triphosphate route.

M L Trimble  

C P Richards

Hydrolysis of tetrapolyphosphate

\[
\begin{align*}
\text{OPOPOPO} + 2 \text{PO}_4^2- & \rightarrow 2 \left[ \text{OPOPO} \right] + \text{PO}_4^3- \\
\text{OPOPOPO} + 2 \text{PO}_4^2- & \rightarrow 4 \text{PO}_4^3-
\end{align*}
\]

Contact time 0 min

30 min

22 h
December 10, 1980

Re: Killing 'em softly; $^{31}$P NMR studies on microorganisms.

Dear Barry:

Usually when NMR spectra of microorganisms are run the cells are re-suspended in liquid medium after centrifugation. They tend to settle down to the bottom of the NMR tube, where because of the rapid depletion of oxygen and nutrients they begin to die.

One strategem taken to avoid this happening is to re-suspend the cells by bubbling oxygen, sometimes with sophisticated spectrometer interlock (1). This is time-consuming in terms of the acquisition of spectra, and does not prevent intermittent deterioration of the sample.

In search of an alternative approach we attempted to set up a continuous flow-through system, using oxygenated medium, but this "perfusion" is much less successful for cells than for organs. The cells block most filters, and this approach is cumbersome.

A simple but viable alternative which keeps the cells alive over a long period, is to embed them in agarose gel supplemented with desired nutrients. In fact, growth of microorganisms in a gel block is a longstanding microbiological technique. Agarose has the virtue of allowing normal diffusion of oxygen and nutrients because the cells are not close-packed. To ensure continuing availability of nutrients and oxygen, a liquid culture medium above the agarose block is bubbled through with either pure oxygen or air.

An illustration of the use of this approach is the increase in the polyphosphate content of resting E. coli incubated in sulfur-free medium (2) over a 24 hr period (Fig.), indicating the continued viability of the cells. Of course, shorter term experiments can also be done, but with added reproducibility utilizing agarose re-suspension. The motion of the cells is, of course, so slow in packed suspensions that embedding them in agarose leads to no net degradation in the quality of spectra.

Sincerely yours,

Lev Jacobson
Jack S. Cohen
Developmental Pharmacology Branch
National Institute of Child Health and Human Development

LJ/JSC;ell
Polyphosphate content as a function of time of a culture of E. coli grown to mid-exponential phase and re-suspended in sulfur-depleted medium (at ca. 10^8) in agarose (0.25%) at 37°C. Oxygen was bubbled through the medium above the agarose block. The 31p NMR peak at -23 ppm was integrated, relative to the final value after 24 hrs set to 100. Spectra were recorded at 109.3 MHz in 3K scans with 0.5 sec delay time.
Heteronuclear two-dimensional NMR is now being applied to some samples of real interest. In this sort of experiment one is typically interested in obtaining high resolution in the proton dimension. For many samples a rather wide spectral width in both the observed nucleus and proton dimensions is needed. This problem becomes more acute at high magnetic field strengths. However, there is a restriction on the resolution placed by the use of large spectral widths. The spectral width in the proton dimension is determined by $1/(2\times$ increment of evolution time) and the resolution is given by equation 1 which is an extension of the results of Maudsley,\[ \Delta \nu (\text{proton}) = \frac{1}{\pi} \left[ \frac{2}{\pi} \left( \frac{1}{\text{increment of evolution time}} \right) \right] \] Wokaun and Ernst (1). The problem is that the resolution in a single slice in the proton dimension is partially determined by the total length of the evolution time but a large spectral width requires a small increment of the evolution time and hence a large number of $t_1$ values. This quickly leads to the storage of more information than the computer can store.

A partial resolution of this problem is to use a phase cycling procedure which mimics quadrature detection. The basic idea is illustrated in Figure 1. In a conventional heteronuclear two-dimensional NMR experiment the cosine of the proton modulation frequencies modulates the observed nucleus signal. The resulting proton spectrum then contains signals which occur at the sum and difference of the proton frequencies relative to the decoupler offset. In the phase cycling approach the experiment alternates between transferring the cosine of the proton frequencies to the real part of the observed signal and the sine to the imaginary part. Some typical data is shown in Figure 1. Figure 1(A) is the proton spectrum obtained from the complex Fourier transform of the cosine modulation, 1(B) is the complex Fourier transform of the sine modulation and 1(C) is their sum. It is seen that there is a good cancellation of images. The important point is that this procedure offers twice the spectral width of the conventional approach for a given increment of the evolution time.

It is important to note that since separate pulse sequences must be used to transfer the cosine and sine modulations the signal to noise gain that occurs in conventional quadrature detection will not be present in this two-dimensional analog. Also, to effectively suppress the presence of a signal at zero frequency to the $F_1$ dimension an additional phase cycling need be used. The pulse sequence actually used to eliminate the zero frequency signal and to give the quadrature transfer is to cycle both the second proton pulse and the observed nucleus pulse through $X, -X, Y, -Y$.

This method is rather similar to the EXORCYCLE approach for J spectroscopy (2). Since the method incorporates both quadrature transfer and elimination of zero fre-
quency signals as well as doubling the spectral width by being able to tell the
difference between the positive and negative sides of the carrier it is dubbed
BICYCLE.


![Diagram](A)

![Diagram](B)

![Diagram](C)

Sincerely,

Philip H. Bolton
Assistant Professor
Dear Barry,

The relationships between reaction rates, rate constants and lifetimes via magnetic resonance have been known for many years.\(^{1,2}\) These have been used to calculate rates and determine mechanisms of exchange between a Lewis acid-base complex and one of its components. The exchange can occur either by dissociation of the complex, in which case the activation enthalpy for exchange equals the heat of dissociation, or by displacement of one species in the complex by excess of free species.

\[
A^* + A - B \rightleftharpoons A^* - B + A
\]

In the latter case the activation enthalpy for exchange will be less than the heat of dissociation. Both types of exchange mechanisms have been observed in various systems. To the best of my knowledge no case has yet been reported where both exchange mechanisms can operate in the same system.

We have investigated the exchange of an excess of either dimethyl sulfide or boron trichloride with boron trichloride-dimethylsulfide complex in methylene chloride and sulfur dioxide solutions via proton, \(^1\)H and \(^11\)B resonance spectroscopy. From the concentration dependence of the exchange rates it was found that dimethyl sulfide exchanges by a dissociation mechanism while boron trichloride exchanges by a displacement mechanism. The rate constants as a function of temperature are shown on the accompanying graph. The enthalpies of activation are 5.0 ± 0.5 kcal/mole for BCl\(_3\) exchange and 20 ± 1 kcal/mole for dimethyl sulfide exchange.


Yours truly,

B. Glavincevski
S. Brownstein
Dear professor Shapiro:

We are interested in the chemistry of 1,6-pyrenequinone (I) and 1,8-pyrenequinone (II). Their preparation by CrO₃ oxidation of pyrene and the separation of the resulting 1:1 mixture of I and II has been described. I and II have been characterized thusfar by IR- and electronic spectra. The 'H-NMR spectra of I and II have not been published. We like to report the 'H-NMR data of I and II (JEOL PFT100, CDCl₃). The 'H-NMR patterns are fully in agreement with the structures. 'H-NMR spectroscopy can more elegantly differentiate between I and II than other analytical techniques used thusfar.

1,6-pyrenequinone (I) assignment

<table>
<thead>
<tr>
<th>δ (ppm)</th>
<th>J (Hz)</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.71</td>
<td>AB</td>
<td>H 2,7</td>
</tr>
<tr>
<td>7.68</td>
<td>J=10.0 Hz</td>
<td>H 3,8</td>
</tr>
<tr>
<td>7.84</td>
<td>AB</td>
<td>H 4,9</td>
</tr>
<tr>
<td>8.49</td>
<td>J=7.6 Hz</td>
<td>H 5,10</td>
</tr>
</tbody>
</table>

1,8-pyrenequinone (II) assignment

<table>
<thead>
<tr>
<th>δ (ppm)</th>
<th>J (Hz)</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.68</td>
<td>AB</td>
<td>H 2,7</td>
</tr>
<tr>
<td>7.68</td>
<td>J=9.7 Hz</td>
<td>H 3,6</td>
</tr>
<tr>
<td>7.67</td>
<td>S</td>
<td>H 4,5</td>
</tr>
<tr>
<td>8.64</td>
<td>S</td>
<td>H 9,10</td>
</tr>
</tbody>
</table>
\(^1\)H NMR spectrum of I and II, ca. 1:1 mixture


CONTINUING EDUCATION PROGRAM ANNOUNCEMENT

TITLE: WORKSHOP ON NUCLEAR MAGNETIC RESONANCE IMAGING

DATE: February 19 & 20, 1981

PLACE: The University of Texas Medical School at Houston
        Department of Radiology and The American Association of
        Physicists in Medicine (AAPM)

CREDIT: 12 Hours - AMA Category I

FEE: $225.00

For further information contact the Office of Continuing Education, The
University of Texas Medical School at Houston, P. O. Box 20708, Houston
Texas 77025, Phone (713) 792-5346.
Dear Dr. Shapiro,

Thank you for your yellow reminder. Last year we published a study on molecular reorientation of CS₂ diluted in alkanes¹, 33S linewidths were used to determine the reorientation correlation time of CS₂ and were measured at 30 MHz on a Bruker WH400 spectrometer.

Recently we ran some further experiments at 15 MHz on our Bruker WP200 spectrometer fitted with a broadband probe. Unfortunately the well-known acoustic ringing occurs at this low frequency, leading to a rolling baseline and precluding accurate linewidth measurement. The ringing persists for approximately 1.5 ms, regardless of the spectral width.

As the 33S linewidth of CS₂ lies in the 300 - 600 Hz range (i.e. \( T_2 = 1 \approx 0.5 \text{ ms} \)) depending upon medium viscosity, most of the 33S FID occurs during probe ringing. Consequently if acquisition is delayed 1.5 ms to eliminate the ringing (successfully used for ¹⁴N at 14 MHz with the same probe) the sensitivity of 33S measurements falls so much that experiments on dilute solutions is impossible. We also tried to acquire the second half of the echo in a 90°-τ-180°-τ-AQ sequence, but if τ is long enough to eliminate the ringing following the 180° pulse, there is no more 33S NMR signal! For the same reason, the sequence proposed by Brooke, Openshaw and Cushley² cannot help when life-times of the ringing and the NMR signal are comparable.

...
We think that only a 15 MHz 33S probe specially designed to eliminate acoustic ringing at the relevant frequency can solve this problem.

Sincerely yours,

B. TIFFON

B. ANCIAN.

1 B. Ancian, B. Tiffon and J.E. Dubois

2 A. Brooke, T.R. Openshaw and R.J. Cushley
Announcement of an International Conference on Conformational Analysis

I am writing to call your attention to an International Conference on Conformational Analysis which will be held at the New England Center on the campus of the University of New Hampshire from June 29 to July 2, 1981.

The Conference is intended to bring together interested scientists from around the world to share information and exchange views. The format of the Conference is such that it should encourage informal discussion. A total of twelve plenary lectures are planned: three each morning for the 3½ days of the Conference. Evenings will be devoted to poster-session presentations by conference participants and afternoons will be free for recreation or informal discussion.

Plenary lectures by the following internationally known authorities have been scheduled and several additional speakers have been contacted.

Prof. F. A. L. Anet, Univ. of California at Los Angeles
Dr. F. A. Bovey, Bell Laboratories
Prof. E. L. Eliel, Univ. of North Carolina
Prof. K. Mislow, Princeton Univ.
Prof. S. Nelsen, Univ. of Wisconsin
Prof. M. Oki, Univ. of Tokyo
Prof. H. Scheraga, Cornell Univ.
Prof. F. Vogtle, Freidrich-Wilhelms Univ.

If anyone should like to receive complete information and registration forms for the Conference, they should contact:

Prof. Gary R. Weisman
University of New Hampshire
Dept. of Chemistry
Durham, NH 03824
Dear Professor Shapiro,

EQUIPMENT FOR SALE

We have the following spectrometers for sale. They have both been maintained by the manufacturers and are in excellent working condition.

**Bruker WH 90, purchased 1973**
- 5mm $^1$H, $^{19}$F probes;
- 10 mm and 15 mm $^{13}$C probes;
- BNC 12 computer, 12K core, teletype, hardware pulse generator.
- Available immediately.
- Price expected in the region of £5,000.

**Jeol FX 100, purchased 1976**
- 1mm, 5mm dual $^1$H/$^{13}$C probes;
- 5mm $^{19}$F probe;
- 10mm $^{13}$C, $^{31}$P, $^{27}$Al probes;
- Variable temperature controller;
- Internal and external 2D lock;
- 24 K computer with cartridge disc-based foreground/background system (added 1980), PG 200 pulse programmer.
- Available April/May 1981.
- Price expected in the region of £35,000.

We would prefer to sell the spectrometers as complete systems, but would consider offers for parts if necessary.

Pricing enquiries should be addressed to Mr S Dwight, Supplies Controller, Unilever Research, Port Sunlight Laboratory, Quarry Road East, Bebington, Wirral, Merseyside L63 3JW, UK. Tel. 051 645 2000 Ext. 681.

Any technical enquiries can be directed to myself at the above address or by telephone to extension 660.

Yours sincerely,

C J CLEMETT
Professor Bernard L. Shapiro  
Department of Chemistry  
Texas A&M University  
College Station, TX 77843

TITLE: NMR Faculty Position

Dear Professor Shapiro:

Our department has a faculty position available for an NMR spectroscopist. The advertisement that is scheduled to appear in the December, 1980 issue of Physics Today is reproduced below:

Applications are invited for a position at the Associate or Assistant Professor level in the Department of Physics, Indiana University-Purdue University at Indianapolis (IUPUI). The applicant should have experience in Nuclear Magnetic Resonance at the Assistant Professor level or equivalent and an interest in biological or medical applications of NMR. It is expected that he or she would initially collaborate with existing groups currently working on high-resolution NMR or imaging. Options exist to interact with ESR groups or the Biophysics division. Preference will be given to persons who can help develop an undergraduate or masters level laboratory in biological physics and are willing to interact with the Indiana University School of Medicine component of IUPUI. Submit applications to Professor B. D. Nageswara Rao, Department of Physics, IUPUI, 1125 E. 38th Street, Indianapolis, Indiana 46205. IUPUI is an Equal Opportunity Employer.

We would appreciate your bringing this to the attention of TAMU readers. The recruitment process is expected to begin by February 1981.

Sincerely yours,

B. D. Nageswara Rao
Yes, Brünnhilde, there really is a high-field NMR alternative:

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- Precise digital plotting with full annotation of spectral parameters and flexibility of hardcopy format.
- The versatile Nicolet spectrometers provide the user with the ability to easily adapt to the newest techniques and experimental configurations.

Some of these are:

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- Automated T1 and T2 measurements.
- Chemical dynamics studies.
- Temperature-programmed experiments.
- 3p experiments on living organs.

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Telephone: 415-969-2076
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- Digital Quadrature Detection
- Oxford SCM Systems
- Programmable Variable Temperature
- Double Precision (32 bit word length)
- Floppy; Moving Head Disc Systems

### FX-60QS:
- CP/MAS
- $^{13}$C, $^{31}$P, $^{29}$Si (examples)
- Routine Liquids/Solid State

### FX-90Q:
- OMNI Probe™ System
- 10mm, 5mm Micro Inserts
- Wide Band ($^1$H to $^{103}$Rh)

### FX-200:
- Dual Frequency Probes
- Broad-Band Probes
- CP/MAS Extension

### FX-270:
- Dual Frequency Probes
- Broad-Band Probes
- "Tilt" Micro Probe