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 Newsletter

No. 241

October, 1978

L. D. Colebrook	Use of an HP 1000 Computer System for NMR.	1
J. T. Gerig	Earthquakes and NMR. Point II	3
H. Booth	Conformational Analysis of Cyclic Compounds Using Variable Temperature ^{13}C NMR Spectroscopy	5
A. Walker	4th Stanford Conference on Molecular Structural Methods in Biological Research, Nov. 10-11, 1978	7
R. H. Cox	Ring Current Effects on ^{13}C Shifts; Postdoctoral Position	10
M. Thorpe	^{13}C Spectra of Four Isomeric Hydroxy-Substituted 2-Acetylaminofluorenes.	12
D. P. Kelly	^{13}C Ipso(α)-SCS and Electron Demand in 1,4-Disubstituted Benzenes.	13
M. L. Maddox	The Configuration of the Methyl Group in Ethyl-1-hydroxy-2-methylbicyclo[3.2.0]hept-6-ene-7-carboxylate	15
P. D. Ellis	Three Research Associates Positions Available and a New Decoupling Sequence	17
E. Oldfield, B. Skarjune and D. Rice	^2H Quadrupolar Echo Studies of Glycolipids and Lipid-Polypeptide Complexes. :	19
E. Oldfield	Widebore 360, 220 and 150 MHz Systems Postdocs	21
U. Henriksson and T. Klason	Erratum to "Order Parameter from ^{13}C Chemical Shift Anisotropy" Appearing in Issue #241 (Oct. 1978)	22
J. P. Fraissard	2nd International Symposium on Magnetic Resonance in Colloid and Interface Science, July 1-8, 1979.	23
P. Servoz-Gavin, J. B. Robert and C. Taieb	4th European Experimental NMR Conference, June 26-29, 1979, Grenoble, France	26
U. Henriksson and T. Klason	Order Parameter from ^{13}C Chemical Anisotropy.	27

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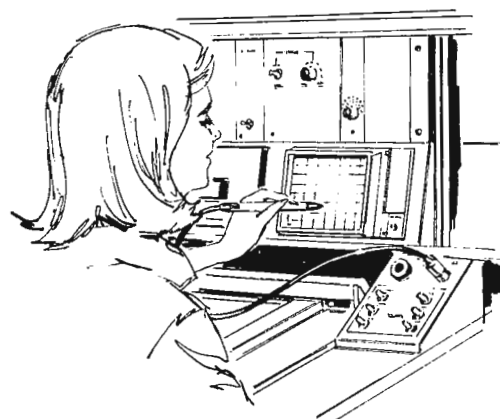
All Newsletter Correspondence, Etc. Should Be Addressed To:

Dr. Bernard L. Shapiro
 Department of Chemistry
 Texas A&M University
 College Station, TX 77843 U.S.A.

AUTHOR INDEX - TAMU NMR NEWSLETTER NO. 241

Booth, H..... 5	Maddox, M. L.....15
Colebrook, L. D..... 1	Oldfield, E.....19
Cox, R. H.....10	Oldfield, E.....21
Ellis, P. D.....17	Rice, D.....19
Fraissard, J. P.....23	Robert, J. B.....26
Gerig, J. T..... 3	Servoz-Gavin, P.....26
Henriksson, U.....22	Skarjune, B.....19
Henriksson, U.....27	Taieb, C.....26
Kelly, D. P.....13	Thorpe, M.....12
Klason, T.....22	Walker, A..... 7
Klason, T.....27	

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DEPARTMENT OF CHEMISTRY



September 5, 1978

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

Dear Barry:

Use of an HP 1000 Computer System for Nmr

Your reminder arrived not long after I had returned to Montreal from Vancouver, where I spent my sabbatical leave working with Laurie Hall, at the University of British Columbia. Much of my time there was spent with the "homebuilt" 270 MHz instrument (TAMU NMR NEWSLETTER, 238, 19 (1978)). We did quite a lot of instrument development, but I also managed to make many proton relaxation (T_1) measurements. I had a very pleasant and profitable stay at UBC.

Before I left Montreal for UBC we took delivery of our new computer system, which replaces our old reliable, but slow and inadequate, Hewlett-Packard 2114A. The new computer is an HP 21MX-E, purchased as an HP 1000, Model 31, package. We have 32K of 16-bit memory, a 4.9 M byte dual disk drive, and an HP 2645A "intelligent" video terminal with dual tape cartridge drives. The new computer is to a large extent software and hardware compatible with the old, so we have been able to transfer some programs, and some peripherals and interface cards, directly from the old system to the new. The computer is interfaced to hobby computer kitset video terminals, and a Teletype. We have built a dual 12-bit DAC, using CMOS IC's, for 'scope display and for plotting with an X-Y recorder. Fortran IV and Assembly languages are currently configured.

Professor B.L. Shapiro

September 5, 1978

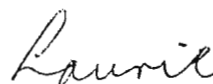
I spent the first part of my leave getting the new system installed and operating. At present it is set up for data acquisition and processing in the pulsed FT mode, and also for CW acquisition. Since we use a homonuclear lock on our modified HA-100, and consequently have dynamic range problems, we use double precision integer data acquisition in the pulsed mode. The data are converted to single precision before Fourier transformation. In the CW mode, data acquisition is synchronized to the recorder movement by using pulses from the recorder x-axis stepping motor as data acquisition flags to signal the computer through its interrupt system. The CW mode is used to digitize spectra for line shape analysis.

The most recent addition to the computer, yet to be installed, is a Writable Control Store and associated software. When this unit is operating, we will be able to program commonly used routines in microcode, which is faster and more efficient than normal Assembly code. The WCS contains 1K words of 24-bit memory. We have obtained a microcoded Fast Fourier Transform package from the HP contributed software library. This should execute very fast. Other candidates for microcoding are phase correction, exponential multiplication, etc.

Program development, from the HP 2645A terminal, is very fast and straightforward. Programs may be written and edited off-line and stored on magnetic tape cartridges, or they may be prepared on-line and stored on disk or on tape cartridges. Ease of program development is a very important consideration to users with a "homebuilt" system who must develop their own software. We find that the HP 1000 is quite comparable to a large time-shared computer in this respect.

Best regards.

Yours sincerely,



L.D. Colebrook
Professor of Chemistry

LDC/ac

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DEPARTMENT OF CHEMISTRY
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September 22, 1978

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

"Earthquakes and NMR. Point II."

Dear Barry:

Seven years ago Professor Roberts provided the first published report of the influence of Californian earthquakes on nmr equipment made by everyone's favorite Californian manufacturer (TAMUNMRN #150, March, 1971) and suggested that perhaps others could supply additional data points. I'm sorry to say that we are now in a position to do so. On August 13 a 5.1 Richter quake with an epicenter approximately six miles from our XL-100/Nicolet system disturbed what was turning into a pleasurable Sunday afternoon. A tremblor of over 30 sec. duration with severe north-south motions and several sharp aftershocks, the event resulted in \$5.5 M damage to the campus and an incredible mess in the chemistry building. There was no permanent relocation of the XL magnet although the consoles were shifted a bit. When electrical service was restored, the system came up smoothly but soon went down and has been subject to an increasingly frustrating series of apparently unrelated component failures-- a diode in the heat exchanger, a 15 V supply in the magnet power supply, op amps in the console, a resistor in the console power supply, and a major, as yet undiagnosed, failure in the Nicolet computer. Perhaps most time consuming in terms of trouble shooting was the dislocation of a connecting pin in the cable from the console to console power supply. In all, nearly six weeks of operating time has been lost and I can't avoid the feeling that we're in for a lot more of lost production. Of course, there's no proof that any of our problems were due to the quake but one wonders what the probability is that all of these "failures of normally reliable parts" would take place nearly simultaneously.

The CFT-20, located on the second floor, suffered damage to the magnet power supply in the form of several resistors being snapped from the circuit card. This was easily repaired and the instrument has been running faultlessly since.

Maybe next time we'll be able to report (1) the resumption of normal operations of the XL-100 and (2) some data obtained therefrom.

Sincerely yours,

Tom

J. T. Gerig
Professor of Chemistry



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Department of Chemistry
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207 Pleasant Street S.E.
Minneapolis, Minnesota 55455

October 3, 1978

Professor Bernard L. Shapiro
Department of Chemistry
College of Sciences
Texas A&M University
College Station, Texas 77843

RE: Postdoctoral Position

Dear Barry:

I currently have a postdoctoral position open immediately for study of NMR relaxation in protein systems. This work will include solid state NMR, cross polarization, and line narrowing experiments, as well as some more straight forward aspects of multinuclear NMR spectroscopy.

My laboratory is currently equipped with two Fourier transform instruments that operate with Varian magnets and Nicolet data systems. Some instrument modification and probe construction is planned.

Anyone interested, with experience in solid state NMR or related areas, may learn more about the details of our program by calling me at (612)373-5575.

Yours truly,

A handwritten signature in cursive script, appearing to read 'Bob'.

Robert G. Bryant
Associate Professor

RGB/mh



University of Nottingham

Department of Chemistry

UNIVERSITY PARK NOTTINGHAM NG7 2RD
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HB/MJS

11th September 1978

Professor B.L. Shapiro,
Department of Chemistry,
Texas A and M University,
College of Science,
College Station,
Texas 77843,
U.S.A.

Dear Professor Shapiro,

Conformational Analysis of Cyclic Compounds
using Variable Temperature ^{13}C NMR Spectroscopy

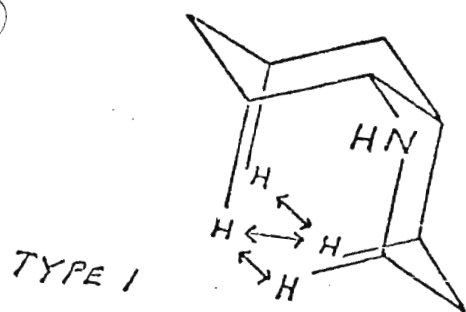
I report briefly some results obtained recently using low temperature ^{13}C NMR¹. We had previously² shown that the conformational equilibrium in cis-decahydroquinoline (1 \rightleftharpoons 2) favoured (2) (93.5% at 199K), in which the nitrogen lone pair can occupy a hindered 'inside' position. Identification of signals due to (1) and (2) used chemical shifts 'calculated' from the shifts in cis-decalin, together with empirical shift parameters for replacement of $-\text{CH}_2-$ by $-\text{NH}-$.

Similar techniques have now shown that (3) is favoured over (4) in the equilibrium in cis-decahydroisoquinoline at 215 K [70% of (3)]. Further, the low-temperature ^{13}C spectrum of (1 \rightleftharpoons 2) in $\text{CDCl}_3/\text{CF}_3\text{CO}_2\text{H}$ showed approximately equal proportions of (5) and (6); a similar experiment using (3 \rightleftharpoons 4) also gave approximately equal proportions of (7) and (8). These results demonstrate that the origin of energy differences between (1) and (2), and between (3) and (4), lies in the difference between H/H interactions and H/lone pair interactions.

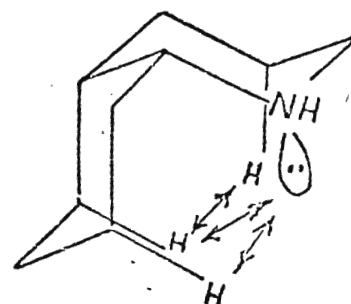
Yours sincerely,

Dr. H. Booth.

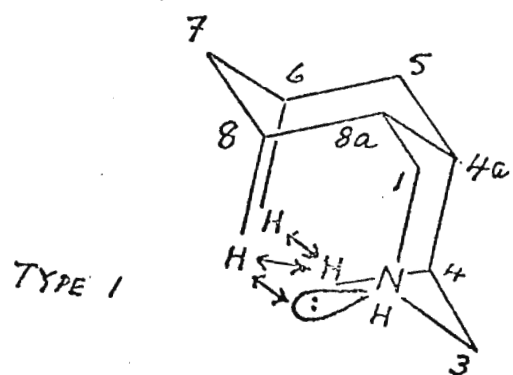
1. H. Booth and J.M. Bailey, J.C.S. Perkin 2 (in press).
2. H. Booth and D.V. Griffiths, J.C.S. Perkin 2, 1973, 842.



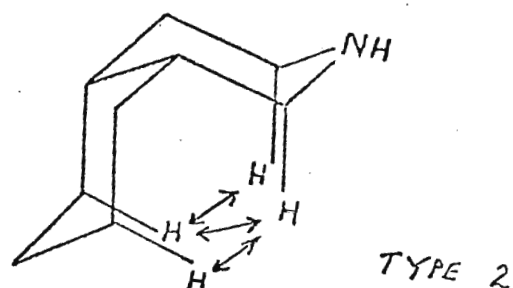
(1)



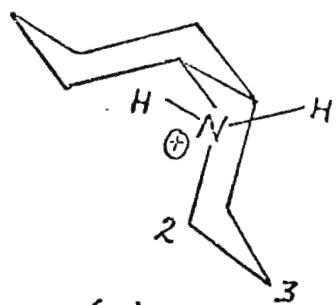
(2)



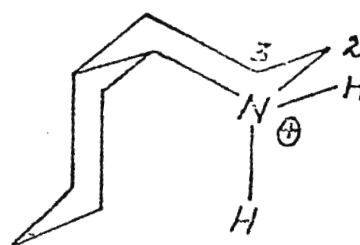
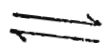
(3)



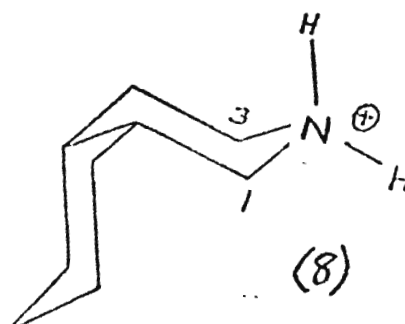
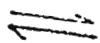
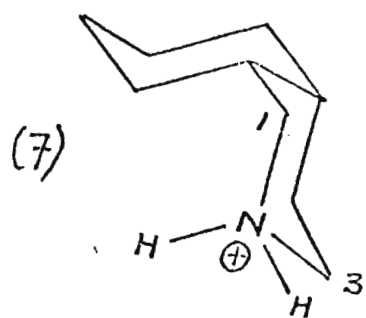
(4)



(5)



(6)



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September 15, 1978

Professor Bernard L. Shapiro
Department of Chemistry
Texas A&M University
College Station, TX 77843
RE: TAMU NMR Newsletter

Dear Professor Shapiro:

The Stanford Magnetic Resonance Laboratory is announcing the Fourth Annual Stanford Conference on Molecular Structural Methods in Biological Research which will be held November 10 and 11, 1978, at the Fairchild Auditorium at Stanford University. The conference will be devoted to recent advances in the solution of biological structural problems by spectroscopic and crystallographic techniques, with a special emphasis on protein structure and dynamics. The conference is sponsored by the Biotechnology Resources Branch of the National Institutes of Health.

Anyone wishing to register or receive further information should contact me at the letterhead address or call at 415/497-6270. A registration fee of \$30 is required to cover the cost of catered luncheons on November 10 and 11 and a banquet dinner on November 10. Closing date for registration is October 20, 1978.

Sincerely,



Alice Walker
Conference Coordinator

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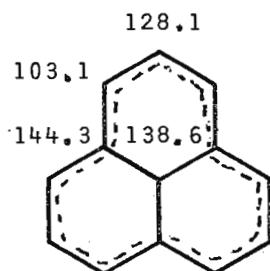
September 10, 1978

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

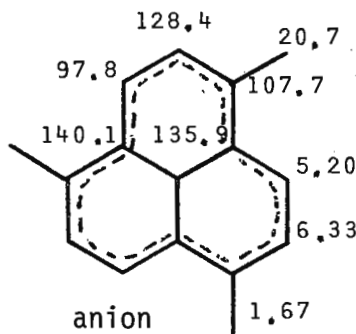
Dear Barry:

Re: Ring Current Effects on ^{13}C Shifts? Postdoctoral Position

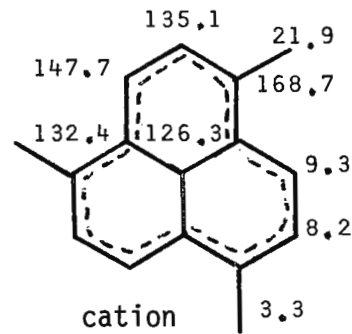
Earlier, in connection with our ion pairing studies, we recorded the ^{13}C spectrum of the phenalenyl anion (Li salt/ d_8 -THF) with the results given below. Because the central carbon shift is upfield from that of the other quaternary carbons, and because in the simple Huckel MO theory the charge on these carbons should be equal, it was thought that the upfield shift might be due to a ring current effect. Furthermore, since the charge on the central carbon is zero, we reasoned that the anion might be behaving as a 14 π -electron periphery and that the corresponding cation might behave as a 12 π -electron periphery and thus, we could examine both a diamagnetic and paramagnetic ring current within the same carbon framework.



anion



anion



cation

Because the phenalenyl cation is not very stable, we have subsequently prepared the 1,4,7-trimethylphenalenyl anion (Li salt/ d_8 -THF), and cation (perchlorate salt/trifluoro acetic acid), and obtained their ^1H and ^{13}C spectra with the results given above. To our initial surprise, the central carbon shift is upfield in both the anion² and cation. After examination of the theory of ring current effects² and the energy levels from Huckel MO theory for the phenalenyl ring system, we believe the results are consistent with the following: (1) because we are dealing with an odd-alternate hydrocarbon, the two "extra" electrons on going from the cation to anion are going into a non-degenerate, non-bonding molecular orbital (thus, there is no splitting of degenerate energy levels as would be the case with a 12-annulene); and (2) therefore both the anion and cation should have identical, diamagnetic ring currents.

Both CNDO and INDO MO calculations reproduce the trends in the chemical shifts with the INDO results giving a slightly better correlation with $\delta_c = -159\rho + 288.5$. The deviations are such that it is difficult to access the ring current effect on the central carbon shifts. Perhaps what is more interesting is that the total difference between the observed shift for the carbons in the cation and the corresponding carbons in the anion is 319.8 ppm. This is in excellent agreement with the predicted value of 320 ppm for a 2 π -electron difference suggested by Spiess and Schneider.

I expect to have an opening for a postdoctoral position starting after October 1, 1978. The conditions are that the person must be a non-US citizen and no more than two years after their Ph.D. Interested persons should forward their resume along with two letters of reference.

Finally, please credit this contribution to Dr. McKinney's account.

Sincerely yours,

Dick

Richard H. Cox
Research Chemist

1. Work done at the University of Georgia.
2. J. A. Pople and K. G. Untch, J. Amer. Chem. Soc., **88**, 4811 (1966).
3. H. Spiess and W. G. Schneider, Tetrahedron Letters, 468 (1961).

Cont'd. from p. 241-12.

δ_C^* for Some Hydroxy-substituted 2-Acetylaminofluorenes

Carbon	1-OH	3-OH	5-OH	7-OH
C ₁	145.21	118.43	115.57	115.96
C ₂	125.42	126.0	137.23	137.01
C ₃	122.22	147.13	117.61	117.83
C ₄	111.35	106.93	122.85	118.58
C ₅	119.74	119.28	152.90	120.03
C ₆	126.22	126.0	113.48	113.97
C ₇	126.61	126.61	127.72	156.52
C ₈	125.08	124.88	115.76	112.15
C ₉	34.30	35.86	36.82	36.44
C ₁₀	130.49	133.57	142.76	142.76
C ₁₁	139.03	137.35	136.07	136.72
C ₁₂	141.19	141.21	126.90	132.48
C ₁₃	142.88	143.61	144.70	144.66
C=O	169.81	168.89	168.07	168.04
CH ₃	23.26	23.72	23.97	23.99

* Solutions in DMSO-d₆ with reference to internal TMS, measured at 25.16 MHz on a Varian XL-100-15 at a concentration of 100 mg/ml.

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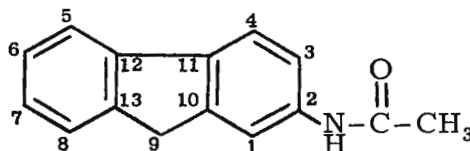
September 14, 1978

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

Title: ^{13}C Spectra of Four Isomeric Hydroxy-Substituted 2-Acetylaminofluorenes

Dear Barry:

During the last few months we have had occasion to determine the ^{13}C spectra of four derivatives of 2-acetylaminofluorene bearing hydroxyl groups at the 1, 3, 5, and 7 positions, respectively.



Using the fluorene data of Stothers, Tan, and Wilson,¹ and substituent constants derived for benzene,² I have arrived at tentative assignments for all four. The assumption was made that a substituent on one ring does not affect the chemical shift of the carbons in the other ring, which is not strictly true. In addition, in two cases the substituents are *ortho* to each other, which introduces additional hazards in making an assignment. And, of course, substituent constants derived for one ring system can hardly be used with certainty for another.

Nevertheless, I have found the approach useful in characterizing these isomers, and in the cases of the two isomers for which we have the proton-coupled spectra (1-OH and 7-OH isomers) the assignments have been consistent with them. Perhaps the data and tentative assignments can be of use to others working with these compounds.

Sincerely,

Martha Thorpe
 Senior Chemist

MT:jkw

1. J. B. Stothers, C. T. Tan, and N. K. Wilson, Org. Magn. Reson., 1977, 9(7), 408-413.
2. J. B. Stothers, "Carbon-13 NMR Spectroscopy," Academic Press, New York, 1972, p 197.

Cont'd. Bottom of p. 241-11.



University of Melbourne
DEPARTMENT OF ORGANIC CHEMISTRY

Parkville, Victoria 3052
25th September, 1978.

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

Dear Professor Shapiro,

¹³C ipso(α)-SCS and Electron Demand in 1,4-Disubstituted Benzenes

Since substituent effects are used routinely in the assignment of ¹³C resonances in aromatic systems it is important to know whether the effects for monosubstituted benzenes published in the texts can be extrapolated to more substituted systems. It has previously been established that para-substituent chemical shifts (SCS) are non-additive in 1,4-disubstituted benzenes, the deviation depending on the nature of the para(4) substituent.¹

We have recently completed a study with Dr. Brownlee's group at La Trobe University of the effect of increasing electron demand upon ipso(α)-SCS in 1,4-disubstituted benzenes. For the substituents Y = MeO, Me, H, F, Cl, Br and CF₃ we have examined the shifts for a large range (25) of substituents X, increasing in electron demand from NMe₂ to ⁺CHCH₃. When the α-SCS [δC4(Y=R) - δC4(Y=H)] are plotted against δC4(Y=H) as a measure of the electron demand of X, a series of lines are obtained as shown in the Figures.

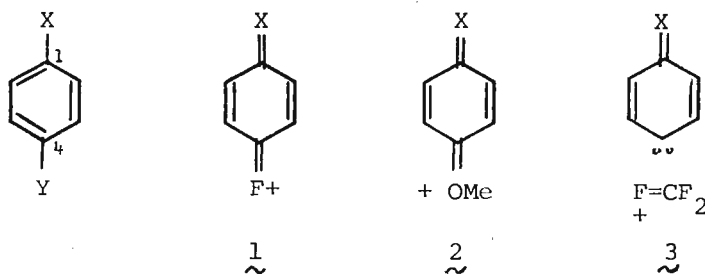
The negative slopes for F, OMe and CF₃ with increasing electron demand are no doubt due mainly to increasing conjugative interaction of these substituents with C4 where the resonance structures 1-3 make an increasing contribution to the ground state of the molecule.

In the case of Me and CF₃ discontinuities occur at X=H which suggest that there is a change in the mechanism of electron supply to the developing electron deficient centre (X) or (less likely) that factors other than electron density are making a major contribution to the shielding of C4.

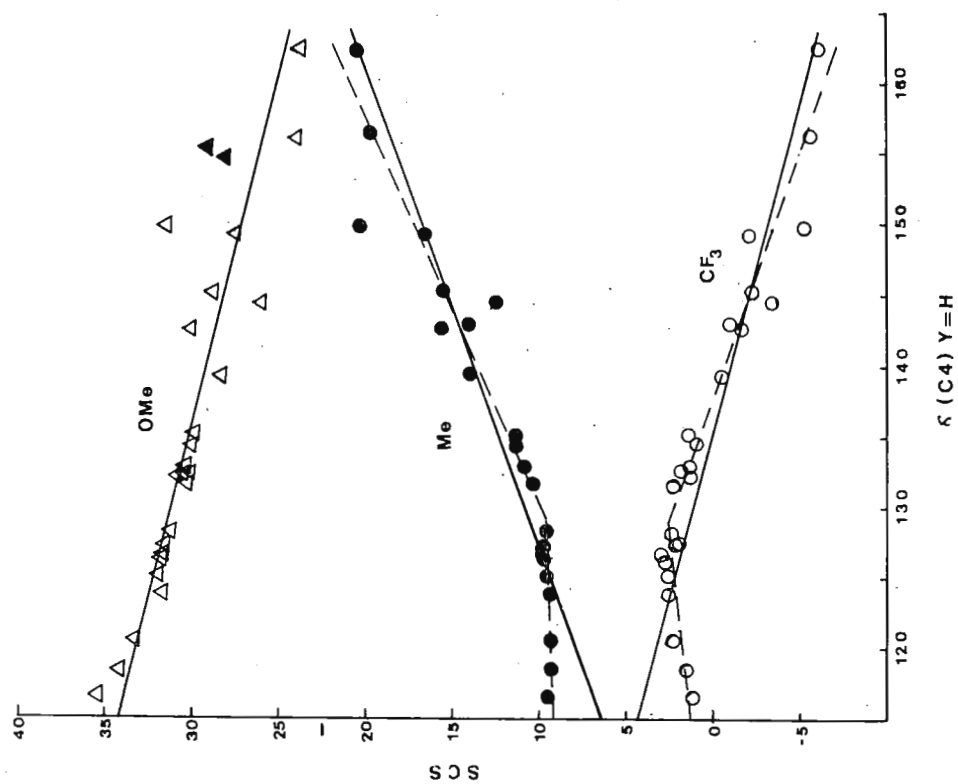
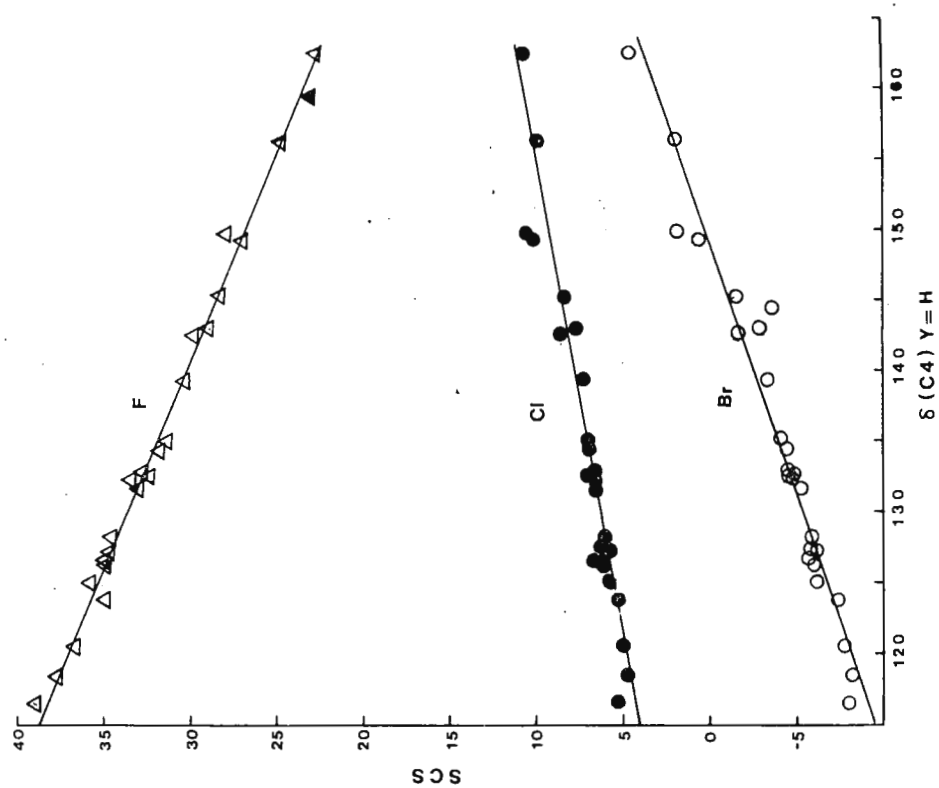
The data presented here should be useful in the assignment of resonances in benzene derivatives and will be submitted to the Australian Journal of Chemistry.

Yours sincerely,


D. P. Kelly.



¹ Bromilow, J., Brownlee, R.T.C., Topsom, R.D., and Taft, R.W., J. Am. Chem. Soc., 1976, 98, 2020.



September 19, 1978
A/R 2057

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

SUBJECT: "The Configuration of the Methyl Group in Ethyl-1-hydroxy-2-Methylbicyclo[3.2.0]hept-6-ene-7-carboxylate"

Dear Barry:

The title compounds were recently synthesized in these laboratories by Dr. Robin Clark and the establishment of the configuration of the 2-methyl group presented an interesting problem. ^{13}C nmr spectroscopy did not yield an immediate solution since the two spectra are quite similar (Table I). Dr. Maria Varasi then measured the ^1H spectra as a function of added $\text{Eu}(\text{fod})_3$ and found that the methyl signals of both isomers gave good, linear plots of $\Delta\delta$ vs $\text{Eu}(\text{fod})_3$ concentration. The slopes of the lines were 155Hz/mg $\text{Eu}(\text{fod})_3$ for I and 48Hz/mg for II. We also measured the ^{13}C spectra at one concentration of shift reagent and those results are included in the Table. With these results, we assigned the structures as shown.

Sincerely yours,



Michael L. Maddox

MM:jg

Attachment

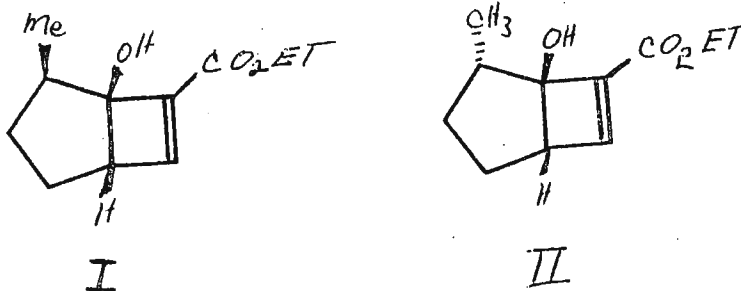


TABLE I
 ^{13}C NMR CHEMICAL SHIFTS^a

<u>Assignment</u>	<u>I</u>	<u>I</u> ^b	<u>II</u>	<u>II</u> ^c
2-CH ₃	13.36	15.18	14.24 ^d	18.04
OCH ₂ CH ₃	14.30	14.63	14.37 ^d	14.60
4	22.40 ^d	24.54	24.32 ^e	25.91
3	31.86 ^d	33.65	32.41 ^e	34.30
2	34.33	38.72	40.96	45.12
5	52.93	55.10	53.87	56.01
OCH ₂	60.30	62.09	60.27	61.93
1	88.07	102.73	88.75	99.67
7	140.73	144.99	138.59	142.55
6	147.78	152.83	148.21	151.98
CO ₂	161.60	165.96	161.96	167.39

a) Measured in CDCl₃ with internal TMS on a Bruker WH-90 at 22.62 MHz

b) With 0.39 eq Eu(fod)₃

c) With 0.29 eq Eu(fod)₃

d,e) Assignment may need to be interchanged

Cont'd. from p. 241-17.

Research Associates Positions in NMR Spectroscopy

The NSF Center in NMR Spectroscopy at the University of South Carolina is seeking highly qualified applicants for three positions within the facility. The salaries for these positions range from \$16,000 to \$17,500. The applicants should have extensive experience in the applications of NMR Spectroscopy. It is anticipated that one of the positions will be filled by a hardware specialist. The duties of the personnel at the center will be divided approximately equally between service and a variety of research programs. The principal instrument of the center will be a Bruker WH-400 NMR spectrometer. This instrument is completely multinuclear, with large tube capability for biological samples. A companion instrument, to which the center has access, is a Bruker WH-200. This instrument, in addition to being multinuclear, is capable of performing high resolution NMR experiments on solids. The starting date for these positions is January 1, 1979. Applicants should send resumés, reprints of published papers, and three letters of reference to: Dr. Paul D. Ellis, Chemistry Department, University of South Carolina, Columbia, South Carolina 29208. The University of South Carolina is an Equal Opportunity/Affirmative Action Employer.



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DEPARTMENT OF CHEMISTRY
(803) 777-5263

October 4, 1978

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

Title: Three Research Associates Positions Available and a New Decoupling Sequence.

Dear Barry:

Needless to say, during the past several weeks my research group and I have been occupying continuous excited states since we heard officially from the National Science Foundation about the Regional NMR Center at the University of South Carolina. We are indeed fortunate to be chosen for this facility, especially in view of the many excellent institutions that applied for similar centers. All that I can say is that we will do everything within our power to provide excellent service to the Eastern region. A brief description of the center is described in the enclosed advertisement for three research associates positions which are available. Further details concerning sample submission and other procedural matters concerning the center will be described in subsequent months.

In a different vein, Dr. Vladimir Basus, Howard Hill, John Waugh, and myself have been working on more efficient decoupling methods for heteronuclear spin decoupling. We have developed a procedure that lowers the power requirements about a factor of 5 (10 watts to 2 watts) while maintaining a decoupling bandwidth of 2 kHz. This bandwidth is defined such that the signal to noise ratio within the bandwidth is not reduced by more than a factor of two. The decoupling sequence involves a combination of chirp and 180°-phase modulation. A manuscript describing the details of this procedure has been accepted in the Journal of Magnetic Resonance and a limited number of preprints are available.

Warmest regards,

A handwritten signature in cursive script that reads "Paul".

Paul D. Ellis
Associate Professor

PDE/bc
Enclosure

Continued Bottom of p. 241-16.

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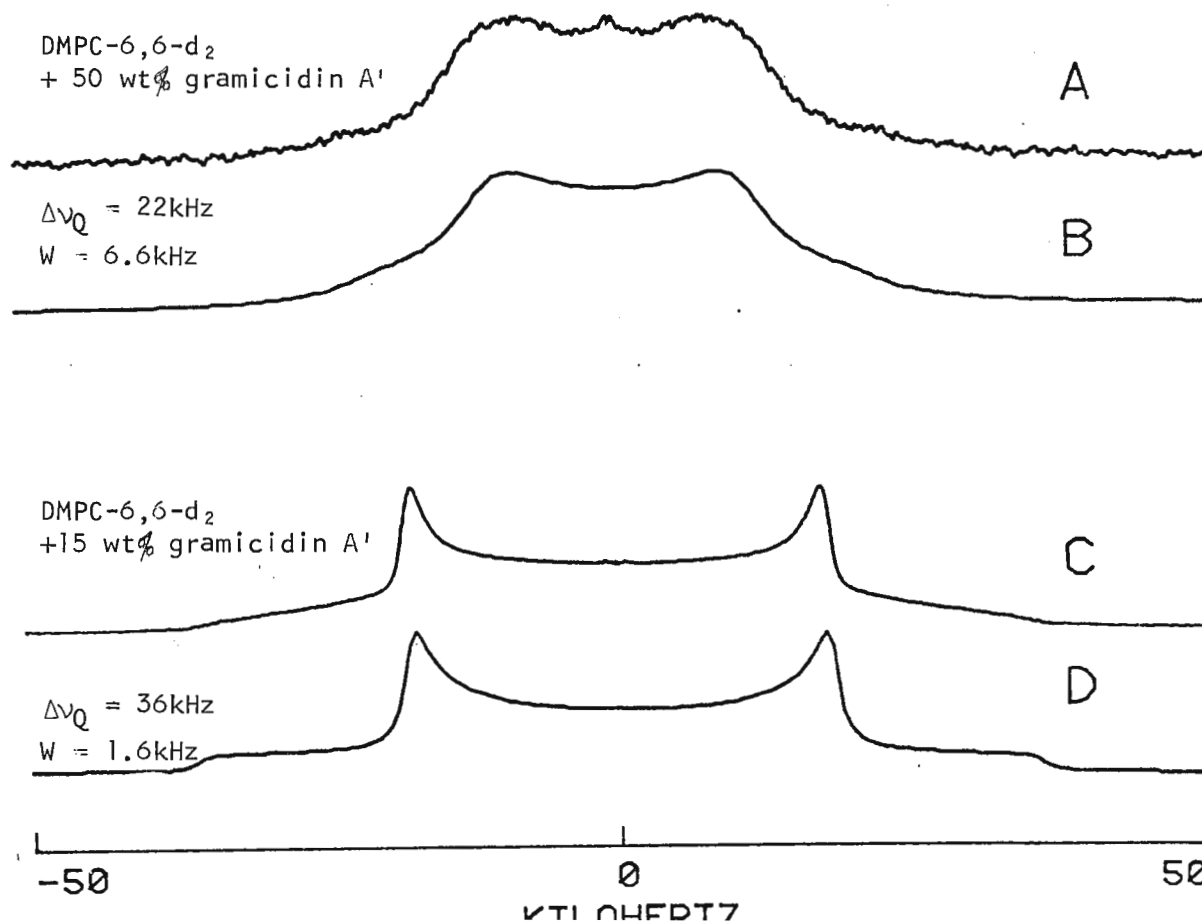
September 28, 1978

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

Dear Professor Shapiro:

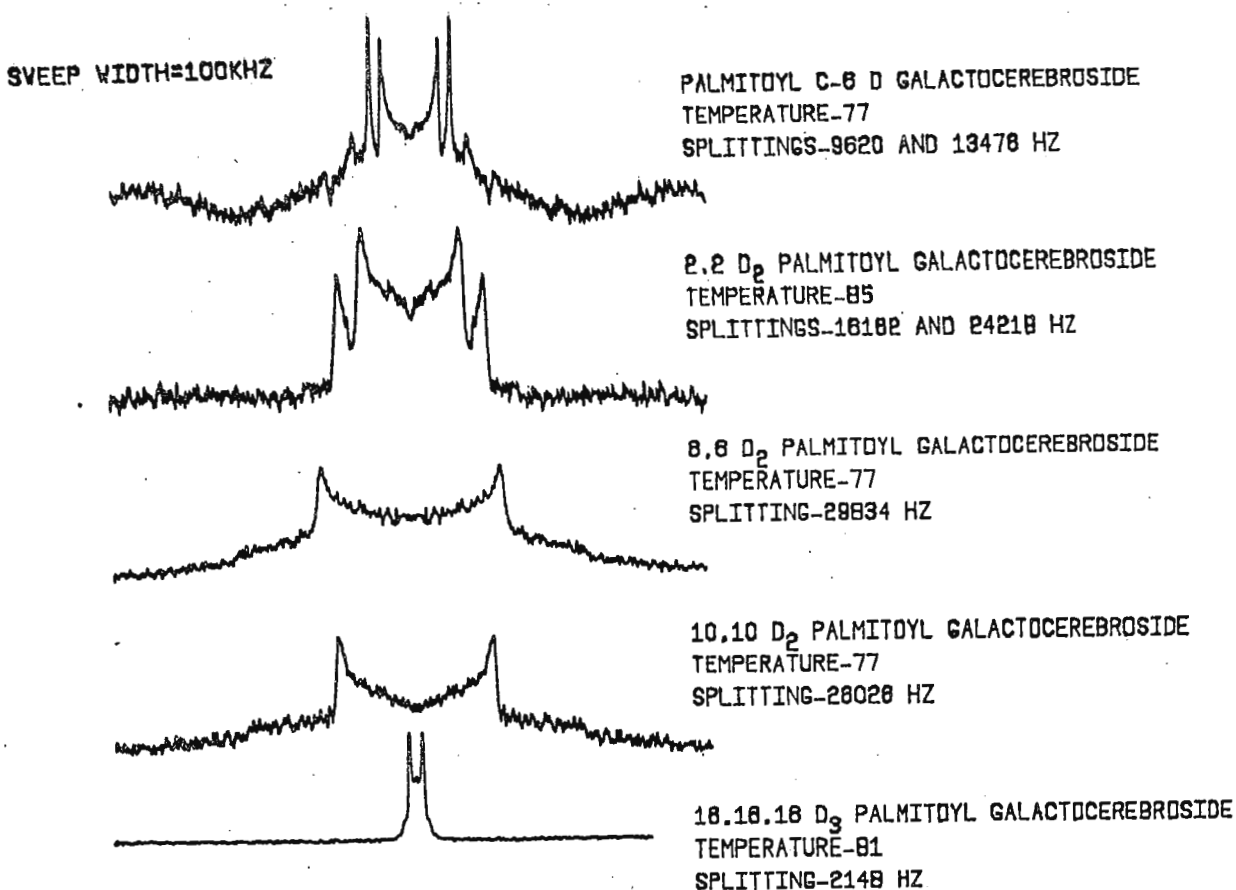
^2H Quadrupolar Echo Studies of Glycolipids and Lipid-Polypeptide Complexes

After reading Ian Smith's recent contribution (TAMUN 239, 31) I thought I might note that in some liquid crystalline systems the quadrupole echo relaxation times, T_{2e} , are exceedingly short, and very small t -delays in the 90° - t - 90° - t -Echo sequence are needed if one is to even see a spectrum! For example, we have observed in the system DMPC-gramicidin A' (DMPC is 1,2-dimyristoyl-3-sn-phosphatidylcholine), where the DMPC is labelled as CD_2 in the 6th position of the 2-chain, that T_{2e} is only about 50 μs ! In the absence of the penta-decapeptide antibiotic gramicidin then T_{2e} is an order of magnitude longer. Since the quadrupole splitting in the spectrum is only about 20 kHz, the effect of the short T_{2e} is to cause a "washing-out" of the quadrupole splitting, as shown in the accompanying Figure.



This type of behavior does not seem to have been observed previously - and it may be of some importance in analyzing the ^2H NMR of intact biological membranes themselves.

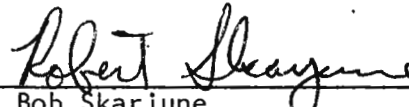
Second, I would like to note that we have recently synthesized a wide range of ^2H -labelled sugar lipids, labelled in both the hydrocarbon chain and headgroup. The results indicate a "bent" conformation for the 2-chain, as in the glycerophospholipids (PE, PC, PA and PS) even though in this case the backbone is sphingosine, and there is no lipid phosphate. The accompanying Figure gives typical results from this type of study.



We are currently investigating the phase behavior of these compounds (cerebrosides), together with their interactions with cholesterol, and some proteins.

Sincerely yours:


Eric Oldfield


Bob Skarjune


Dave Rice

University of Illinois at Urbana-Champaign

School of Chemical Sciences

Urbana, Illinois 61801

September 28, 1978

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

Dear Barry:

Widebore 360, 220 and 150 MHz Systems Postdocs

I am pleased to announce the forthcoming delivery (January, 1979) of an Oxford wide-bore 360 MHz system to my laboratory, which will complement our existing home-built widebore 220 and 150 MHz spectrometers (1,2). The system will of course be fully multinuclear and have cross-polarization and magic-angle capabilities.

I shall have several postdoctoral positions available for work on these instruments, in the following areas:

1) Quadrupole-echo studies of specifically ^2H -labelled membranes. Topics of interest here include the study of protein-lipid interaction in for example the cytochrome oxidase system (3,4) and relaxation studies in liquid crystals.

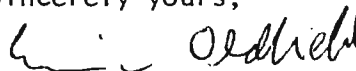
2) Phosphorus-31 NMR studies of protein-lipid interaction in both model and biological membrane systems.

3) High-resolution ^{13}C NMR spectra of protein crystals using high-power decoupling and magic-angle sample-spinning techniques, together with studies of protein-structure in solution using large-sample sideways-spinning tube probes.

4) Development of a LN_2 and then a LHe cooled-coil probe for room temperature high resolution NMR. The idea here is, of course, to reduce the thermal noise from the probe (and preamp).

Applications should consist of a curriculum vitae, list of publications, and names and address of three references.

Sincerely yours,



Eric Oldfield
Assistant Professor of Chemistry
(217-333-3374)

- (1) E. Oldfield and M. Meadows, J. Magn. Res., in press (August, 78).
- (2) E. Oldfield, M. Meadows, D. Rice, and R. Jacobs (1978) Biochemistry 17, 2727-2740.
- (3) S. Kang, H. S. Gutowsky, J. C. Hshung, R. Jacobs, T. E. King, D. Rice, and E. Oldfield, to be published in Biochemistry.
- (4) E. Oldfield, R. Gilmore, M. Glaser, H. S. Gutowsky, J. C. Hshung, S. Y. Kang, T. E. King, M. Meadows, and D. Rice (1978) Proc. Natl. Acad. Sci. U.S.A., in press (October issue).

DIVISION OF PHYSICAL CHEMISTRY
THE ROYAL INSTITUTE OF TECHNOLOGY

S-100 44 STOCKHOLM 70

SWEDEN

Cable address: Technology

Stockholm, September 19, 1978

Professor B L Shapiro
Dept of Chemistry
Texas A&M University
COLLEGE STATION
TX 77843 U S A

Erratum to "Order Parameter from ^{13}C Chemical Shift Anisotropy"

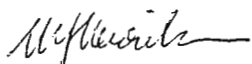
Dear Professor Shapiro,

The correct expression for the Hamiltonian for the case of an axially symmetric shielding tensor should be

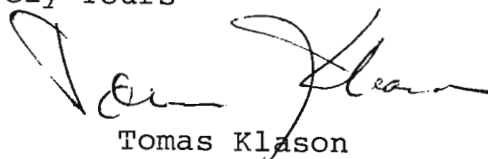
$$H = -\gamma \hbar B_0 I_z [1 - \sigma - (3 \cos^2 \beta_{DL} - 1) \frac{1}{3} (\sigma_{\parallel} - \sigma_{\perp}) \cdot S]$$

and this results in a positive sign of the reported order parameter for C_6H_6 solubilized in the hexagonal phase in the system CTAB- H_2O

Sincerely Yours



Ulf Henriksson



Tomas Klason

THE SECOND INTERNATIONAL SYMPOSIUM ON MAGNETIC RESONANCE IN COLLOID AND INTERFACE SCIENCE

FRANCE, July 1-8, 1979

First circular

We have pleasure in announcing the Second International Symposium on Magnetic Resonance in Colloid and Interface Science to be held in France, July 1-8, 1979.

At the time of printing this Symposium is cosponsored by the :

*Division of Colloid and Surface Chemistry of the American Chemical Society,
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Comparison with results obtained by other techniques will be appreciated.

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C. TAUPIN (Paris)	

PUBLICATION

The plenary lectures, contributed papers and discussions will be published in the Proceedings of the Symposium.

FURTHER INFORMATION

Those interested in the Symposium are requested to complete and return the enclosed post-card before September 15, 1978, to ensure reception of the second circular containing detailed information (December 1978).

DEADLINES

January 15, 1979 for abstract (no more 300 words),
March 15, 1979 for manuscript.

CORRESPONDENCE

All correspondence concerning the Symposium should be addressed to

Professor FRAISSARD
Université P. et M. CURIE, Tour 55
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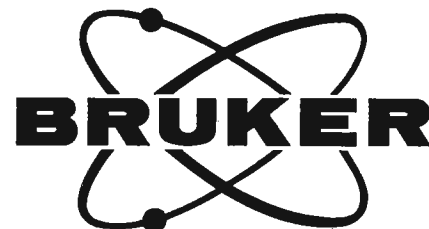
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Dr SHAPIRO

Department of Chemistry
Texas A. & M. University
College Station, Texas
U.S.A.

Dear Dr Shapiro,

This letter is to announce the 4 th European Experimental N M R Conference which will be held at the Autrans Olympic village , from June 26 to June 29 1979. Autrans site of the 1968 Winter Olympic games is located 30 km south of Grenoble at an altitude of 1100 m.

The general scope of the Conference will concern the experimental aspects of N.M.R.. The topics to be covered will include : Very high fields; Two dimensional Fourier transformation; Spin mapping; Solid state N M R; Polymers study; Anisotropy of N M R parameters; Relaxation; Techniques in biochemical or biomedical applications; Multiple quantum transitions; Liquid crystals.

The scientific program will consist mainly of invited lectures and contributed papers presented as posters. A small number of participants will however be invited by the organizing committee (R. FREEMAN; M.J.A. De BIE; P. DIEHL; S. FORSEN; K. SCHAUMBURG; P. SERVOZ-GAVIN; D. ZIESSOW) to present their material in talks. This selection will be made upon study of the abstracts received after the mailing of the second circular.

An exhibition of N M R instruments will be held during the whole period of the Conference.

For further information write to :

P. SERVOZ-GAVIN
4 th EENC
Section de Résonance Magnétique
C.E.N.Grenoble 85 X
38041 GRENOBLE CEDEX
France, Tel. (76) 97-41-11.

For the local organizing committee

P. SERVOZ-GAVIN

J.B. ROBERT

C. TAIEB.



Stockholm, August 29, 1978

Professor B L Shapiro
Dept of Chemistry, Texas A&M UniversityORDER PARAMETER FROM ^{13}C CHEMICAL ANISOTROPY

Dear Professor Shapiro,

In an earlier note (1) we have reported ^2H quadrupolar splittings from C_6D_6 and C_6D_{12} solubilized in aqueous micellar solutions and the hexagonal liquid crystalline phase of hexadecyltrimethylammonium bromide (CTAB). From these splittings the absolute value of the order parameter for the solubilizate has been obtained (2).

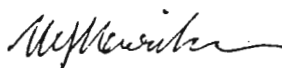
In order to determine the sign of the order parameter we have also studied the ^{13}C chemical shift anisotropy for benzene in the hexagonal phase (34.3% CTAB, 65.7% H_2O . Mole ratio $\text{C}_6\text{H}_6/\text{CTAB} = 0.6$). The observed spectrum is shown in the figure. Using the chemical shift anisotropy $\sigma_{\parallel} - \sigma_{\perp} = 180$ ppm for benzene and the Hamiltonian for the case of an axially symmetric shielding tensor

$$H = -\gamma \hbar B_0 I_z [1 - \sigma + (3 \cos^2 \beta_{DL} - 1) \frac{1}{3} (\sigma_{\parallel} - \sigma_{\perp}) \cdot S]$$

where S is the order parameter for the orientation of the C_6 -axis of the benzene molecule, we obtain $S = -0.071$.

- (1) TAMU NMR Newsletter 228, 33 (1977).
(2) Henriksson, U., Klason, T., Ödberg, L. and Eriksson, J.C. Chem. Phys. Lett. 52, 554 (1977).

Sincerely yours

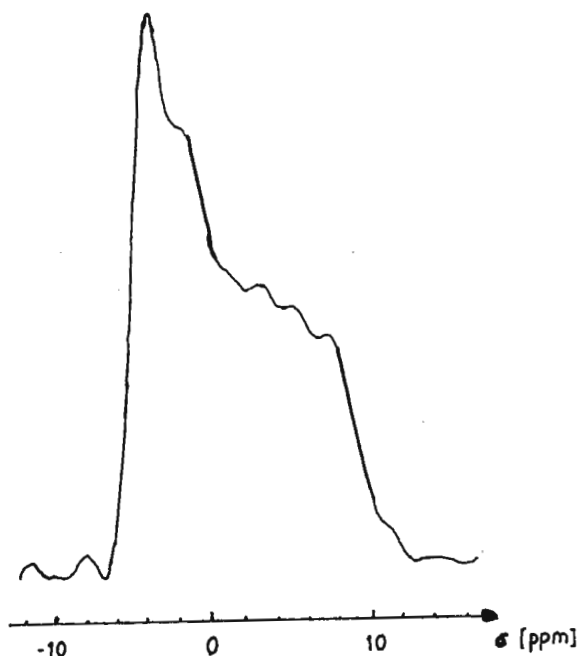


Ulf Henriksson



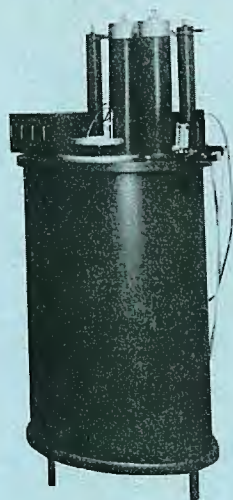
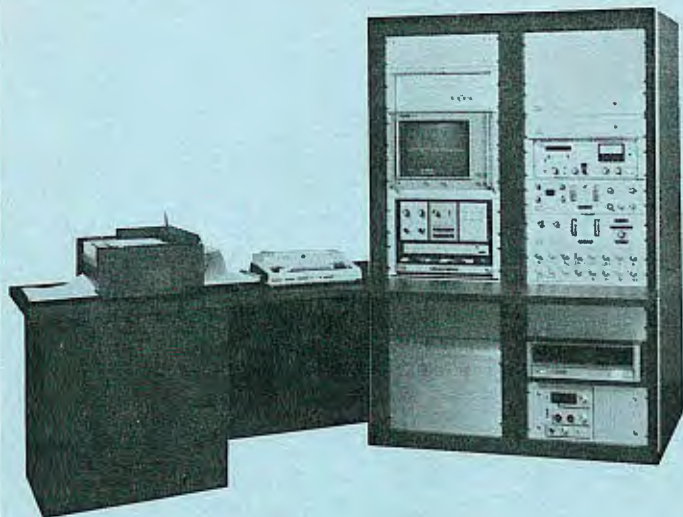
Tomas Klason

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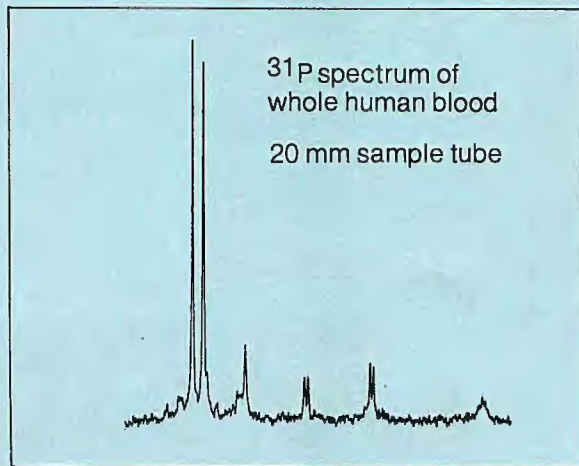
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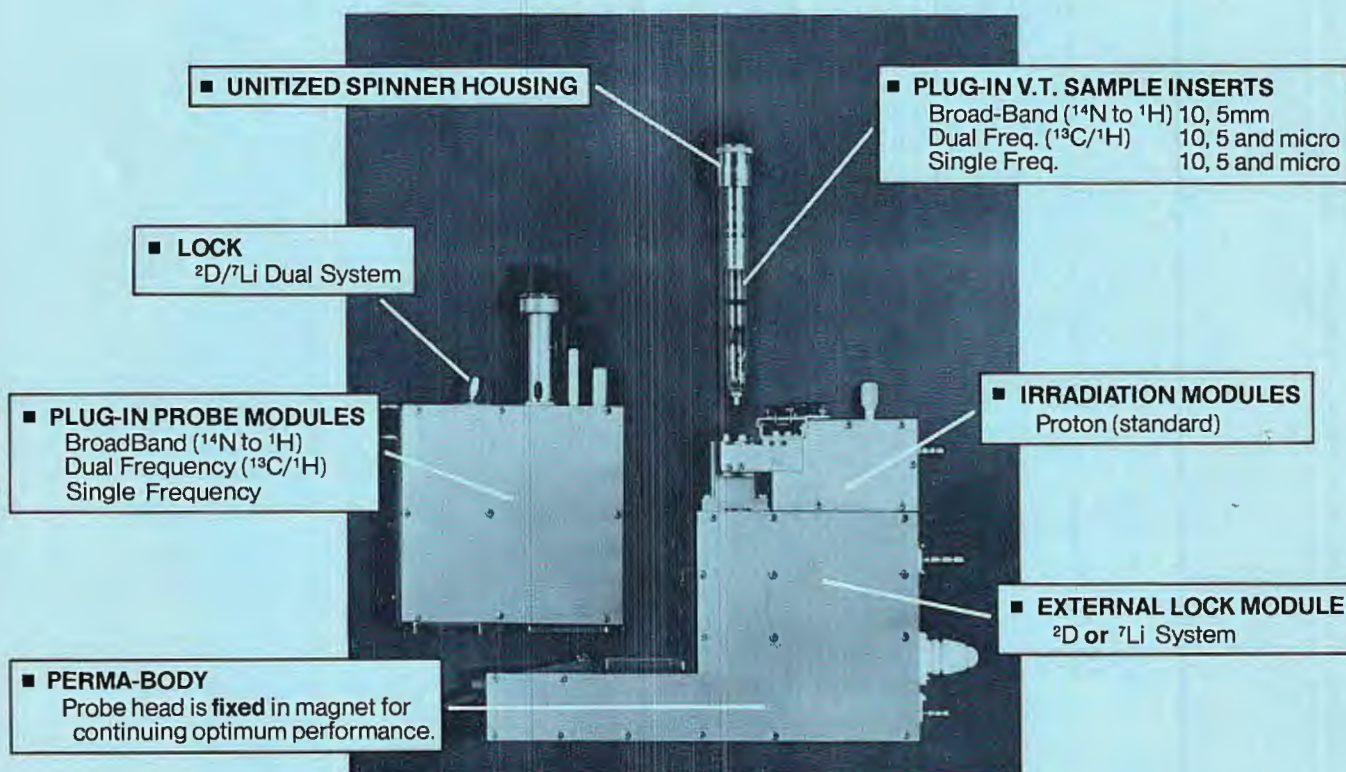
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In the continuing development of the FX series, JEOL now offers a compact, 90 MHz, broad-band, FT NMR System at a cost comparable to the lower frequency systems. The "OMNI PROBE"™ system is designed to provide the highest performance throughout the **entire** observation range.



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