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NMR
NEWSLETTER

No. 282

March, 1982

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DEADLINE DATES:	No. 283	5 April 1982
	No. 284	3 May 1982

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. 282

M bil Research and Development Corporation

January 8, 1982

RESEARCH DEPARTMENT
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J.J. WISE
MANAGER
FIELD RESEARCH LABORATORY

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

Re: OBSERVATION OF ANOMALOUS LINE WIDTH VARIATION WHEN SETTING THE MAGIC ANGLE USING A QUADRUPOLAR NUCLIDE

Dear Barry:

I just received our second issue of the TAMU NMR Newsletter. It has a lot of interesting material, and I wish we had participated earlier.

We recently installed a JEOL FX-60QS spectrometer, and I was greatly interested in Gary Maciel's contribution concerning the use of the Br-79 resonance in KBr to set the magic angle for C-13 measurements. Fortunately, I can use this method since the instrument has a 50 kHz spectral width. Since the lowest frequency of this spectrometer is 15.00 MHz, this spectral width enables me to observe Br-79, even though the resonance is not centered. The method works very well on the FX-60QS.

While adjusting the spinner through the magic angle and carefully plotting the Br-79 central peak, I made a curious observation which I haven't been able to explain. The line width appears to be at a maximum at the magic angle, and the peak intensity is at a minimum. This is shown below:

Angle (degrees)	Peak Height (relative)	Line Width (Hz)
55.61	130	80.1
55.32	123	84.0
55.03	117	93.1
54.74	103	110.3
54.45	112	93.2
54.16	119	83.5
53.87	122	80.5

The KBr was from Mallinckrodt, infrared grade. It was mixed with hexamethyl benzene.

It would be interesting to explain this observation so as to be able to understand spectral parameters of MAS of quadrupolar nuclei. I am sure that we will see many effects from quadrupolar nuclei which do not show up for spin - $\frac{1}{2}$ nuclei.

Sincerely,

Don

D. E. Woessner

DEW:daf

The 6th European Experimental NMR Conference will be held in Haute-Nendaz, Switzerland, from September 14th to 17th, 1982. As is usual for these meetings, the emphasis will be on new techniques rather than on applications of nuclear magnetic resonance. The scientific programme will consist of talks by invited speakers covering the fields of spin imaging, two-dimensional spectroscopy, relaxation studies, new instrumental techniques, applications to medicine and biology and high resolution NMR in the solid-state. There will also be poster sessions and a scientific instrument exhibition. Bursaries are available to help students participate in the meeting. The Chairman is Professor Dieter Ziessow, Technical University of Berlin. Haute-Nendaz is a mountain village above the town of Sion which in turn is served by frequent trains from Geneva.

TECHNISCHE HOGESCHOOL DELFT
Laboratorium voor Technische Natuurkunde

Bereikbaar met buslijn 60 en 63 (station N.S.-Delft)

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

Uw kenmerk	Uw brief van	Ons kenmerk	Datum	Delft, Lorentzweg 1
		RW/MM/079	25 February 1982	Doorkiesnummer (015) 78

Onderwerp

Dear professor Shapiro,

The use of DNP for fast coal characterization with ^{13}C NMR

Besides a.o. protons and ^{13}C atoms coal contains a lot of radicals, typically 10^{19} per gram. It is well-known that in solids containing radicals the nuclear polarization can be enhanced by irradiating near the larmor frequency of the electrons. This is due to the Dynamic Nuclear Polarization (DNP) effect (1). Indeed in coal a considerable proton enhancement has been observed (2). It is also known that the ^{13}C spectrum of a coal can be used for coal characterization, as the observed aromaticity depends on the coal rank. However, usually the measuring time of such a spectrum is rather long, an hour or more. The implication of DNP opens the possibility of fast coal characterization. This can be achieved in two ways:
(i) by firstly enhancing the proton polarization and then transferring this polarization towards the ^{13}C spin species via Cross-Polarization (CP);
(ii) by enhancing the ^{13}C signal directly, and measuring the ^{13}C spectrum via a standard FID experiment.
Fig. 1a shows the ^{13}C spectrum of a low volatile bituminous coal, as obtained with the normal CP method. Fig. 1b shows the same experiment, but now the proton polarization is enhanced by a factor 20

LABORATORIUM VOOR
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~~VERVOLG~~BLAD No.
BRIEF No. 079 d.d. 25 February 1982

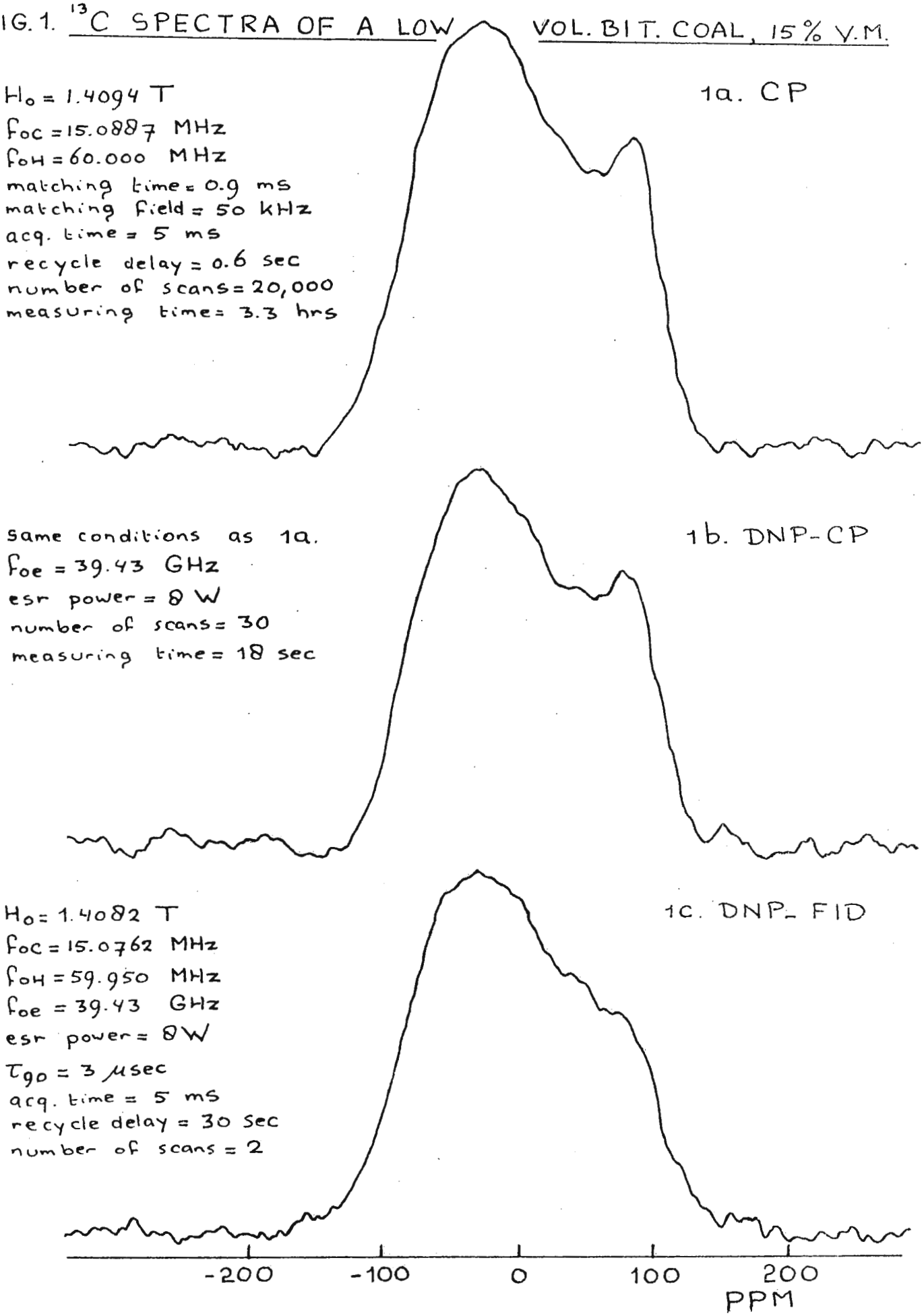
using DNP. We see that in 18 sec. now a same signal-to-noise ratio is obtained as in the more than three hours it took to measure the CP spectrum without DNP! Fig. 1c shows the directly enhanced ^{13}C spectrum using a DNP-FID experiment. Here only 2 scans are needed to obtain an appreciable signal-to-noise ratio; we estimated the ^{13}C enhancement factor to be about 200. However, a disadvantage of the latter method is that the spectrum is distorted; comparing fig. 1c with fig. 1a and 1b, we see that the aliphatic part of the signal is suppressed. This is probably due to the fact that the radicals are in the aromatic region of the coal, and ^{13}C - ^{13}C spin diffusion is not capable of transferring the polarization enhancement into the aliphatic region. Nevertheless, a fast coal characterization becomes feasible now, especially with the DNP-CP method, and also investigations of the coal structure with variable matching times experiments etc. become less time-consuming. Moreover, DNP can also be used in other solids by implanting them with radicals. Finally, if wanted the DNP-CP experiments can be combined with magic angle spinning.
Publications about the various results and the experimental set-up are in preparation.

Yours sincerely,

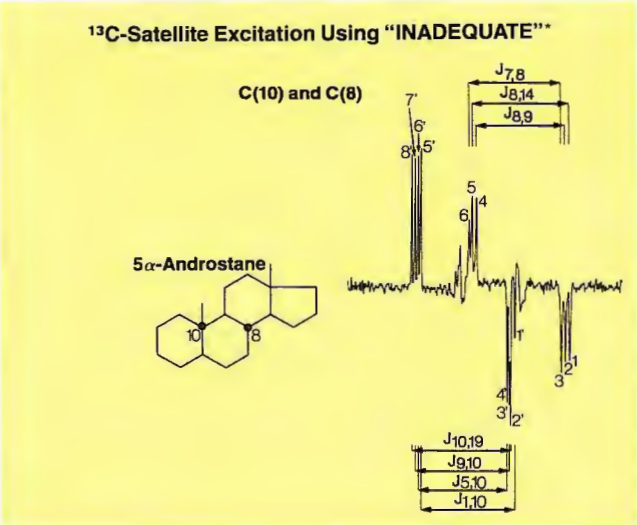
R.A. Wind M.J. Duijvestijn J. Smidt

1. A. Abragam and M. Goldman, Rep. Progr. Phys. 41, 395 (1978)
2. R.A. Wind, J. Trommel and J. Smidt, FUEL 58, 900 (1979)

FIG. 1. ^{13}C SPECTRA OF A LOW VOL. BIT. COAL, 15% V.M.

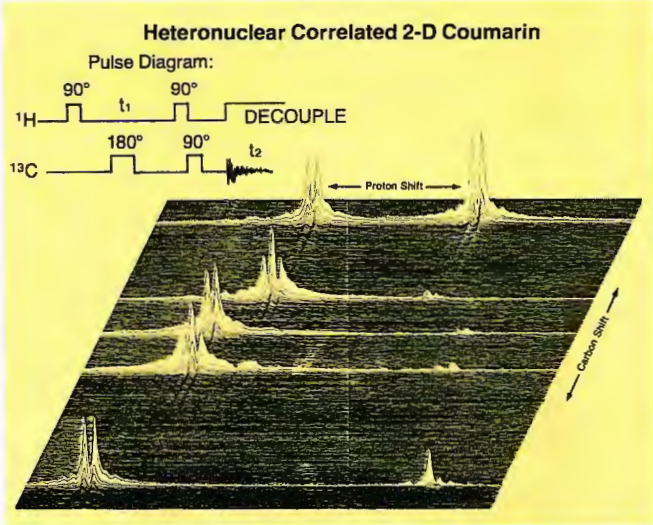


We produced these spectra—



Expansion of the partial INADEQUATE spectrum of 5α-androstane, showing overlapping ^{13}C satellites of carbon 8 and 10. Note the efficiency of center-band cancellation resulting from the hardware stability and the software flexibility of the XL-200 pulse programmer. Assignments shown are the result of the "COSMIC" automatic analysis program on the XL-200.

*A. Bax, R. Freeman and S.P. Kempsell, *JACS*, **102**, 4849 (1980).



Heteronuclear Correlated 2-D NMR on coumarin. Presence of a resonance indicates presence of a C-H bond. The sub-splittings along the proton direction are the homonuclear ^{1}H-^{1}H splittings, even though the experiment is ^{13}C observe. The phase cycling employed in the pulse sequence allows quadrature operation in both frequency domains.

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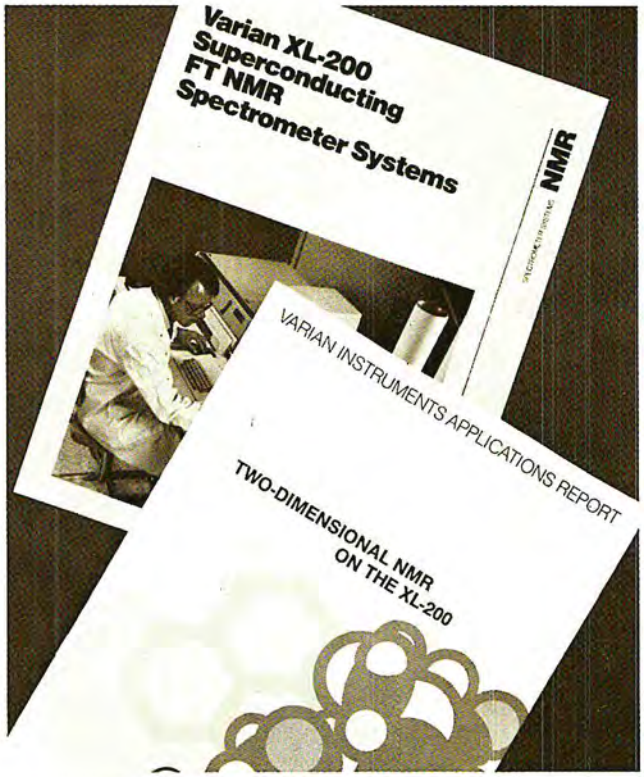

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February 10, 1982

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

Isomers of N-3-(trifluoromethyl)phenyl-3-chloro-4-chloromethyl-2-pyrrolidone

Dear Barry:

The proton NMR spectrum of N-phenyl-2-pyrrolidone, was analyzed by Raisanen et al (Suomen Kemistilehti, 44, 354 (1971). They reported that the cis vicinal coupling, (J_{34})cis (8.8 Hz), is larger than the trans vicinal coupling, (J_{34})trans (6.7 and 7.6 Hz). We have studied the proton and carbon NMR spectra of the cis and trans isomers of N-3-trifluoromethyl-phenyl-3-chloro-4-chloromethyl-2-pyrrolidone. The vicinal H-H coupling constants were found to be 8.7 and 6.0 Hz. Based on Raisanen's studies, we would assign the 8.7 Hz coupling to the cis isomer and 6.0 Hz coupling to the trans isomer.

The carbon shifts for the chloromethyl groups are 43.06 (Isomer having vicinal H-H coupling of 8.7 Hz) and 41.83 ppm (Isomer having vicinal H-H coupling of 6.0 Hz). This implies that the chloromethyl group resonates at lower field when it is cis to chlorine than trans to chlorine. However, from the low temperature carbon-13 NMR spectrum of chloro-cyclohexane, Suttotin and Sergeyev (JACS, 97, 1080 (1975) reported that the steric γ shift for chlorine ($\delta eq - \delta ax$) is +6.5 ppm. Further work is now in progress to study the γ steric shifts in pyrrolidones.

Sincerely,

CKTseng

C. K. Tseng

D J Bowler

D. J. Bowler

mn

The Wellcome Foundation Ltd Langley Court
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BMNC/82/1

11th January 1982

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

Dear Professor Shapiro

A New Angle on Spinning

We have recently designed an apparatus to allow us to perform titrations inside the n.m.r. tube on our old Bruker HX-90 which will also be applicable for use on our Bruker WM-360. As it is necessary to mix the titrant into the solution and as it would also be nice to spin the sample at the same time, we came up with the idea of not spinning the tube in the usual manner but spinning the solution using a paddle made from a glass capillary tube suspended concentrically and held outside the receiver coil. The capillary has a turbine fixed to it above the n.m.r. cap (through which it passes) and the turbine is rotated using a glass nozzle attached to the conventional spinner air/N_2 supply and fixed to the normal probe housing. A typical result is shown in the attached figure. The top trace is ethyl benzene at 90 MHz, non-spinning, the centre trace arises from spinning the solution and the lowest trace from spinning the whole assembly including the tube. The result is more than adequate for titration studies and it is possible to spot one other advantage. Because the solution is not being rotated in a circular fashion there is no single modulation frequency and thus negligible spinning sidebands. This is more magic than magic-angle spinning! Further details are available from the undersigned.

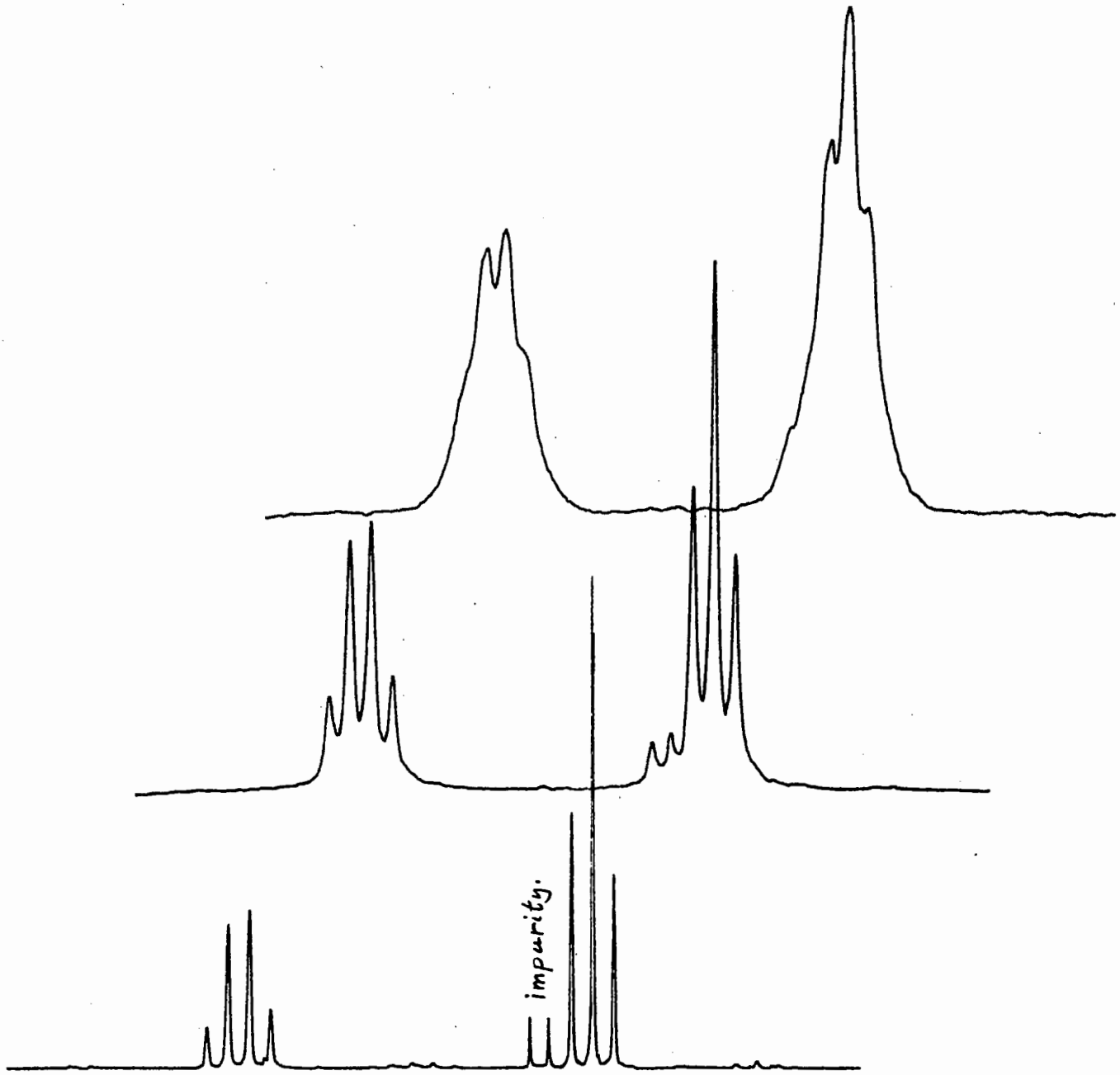
Yours sincerely

John

Tony

J.C. Lindon

A.G. Ferrige


impurity.

McMASTER UNIVERSITY
Department of Chemistry
1280 Main Street West, Hamilton, Ontario, L8S 4M1
Telephone: 525-9140

January 29, 1982

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

Dear Dr. Shapiro

^{61}Ni NMR Study of Some d^{10} Nickel Complexes.

In order to help establish the ranges of ^{61}Ni NMR chemical shifts, coupling constants, relaxation times and natural line widths, we have undertaken a program aimed at assessing the viability of natural abundance ^{61}Ni NMR as a structural probe. Our initial studies involve a series of d^{10}, tetrahedral NiL_4 complexes which yielded the following chemical shift data.

$Ni(PF_3)_4$	-929.1 ppm
$Ni[(P(OMe)_3]_4$	-742.2 ppm
$Ni[P(OEt)_3]_4$	-703.0 ppm
$Ni(CO)_4$	0 ppm
$Ni(PCl_3)_4$	266.9 ppm

Figure 1 clearly shows the phosphorus and fluorine coupling in $Ni(PF_3)_4$. A fuller account will appear in J. Mag. Res. shortly.

Sincerely

B.G. Sayer G.J. Schrobilgen N. Hao M.J. McGlinchey

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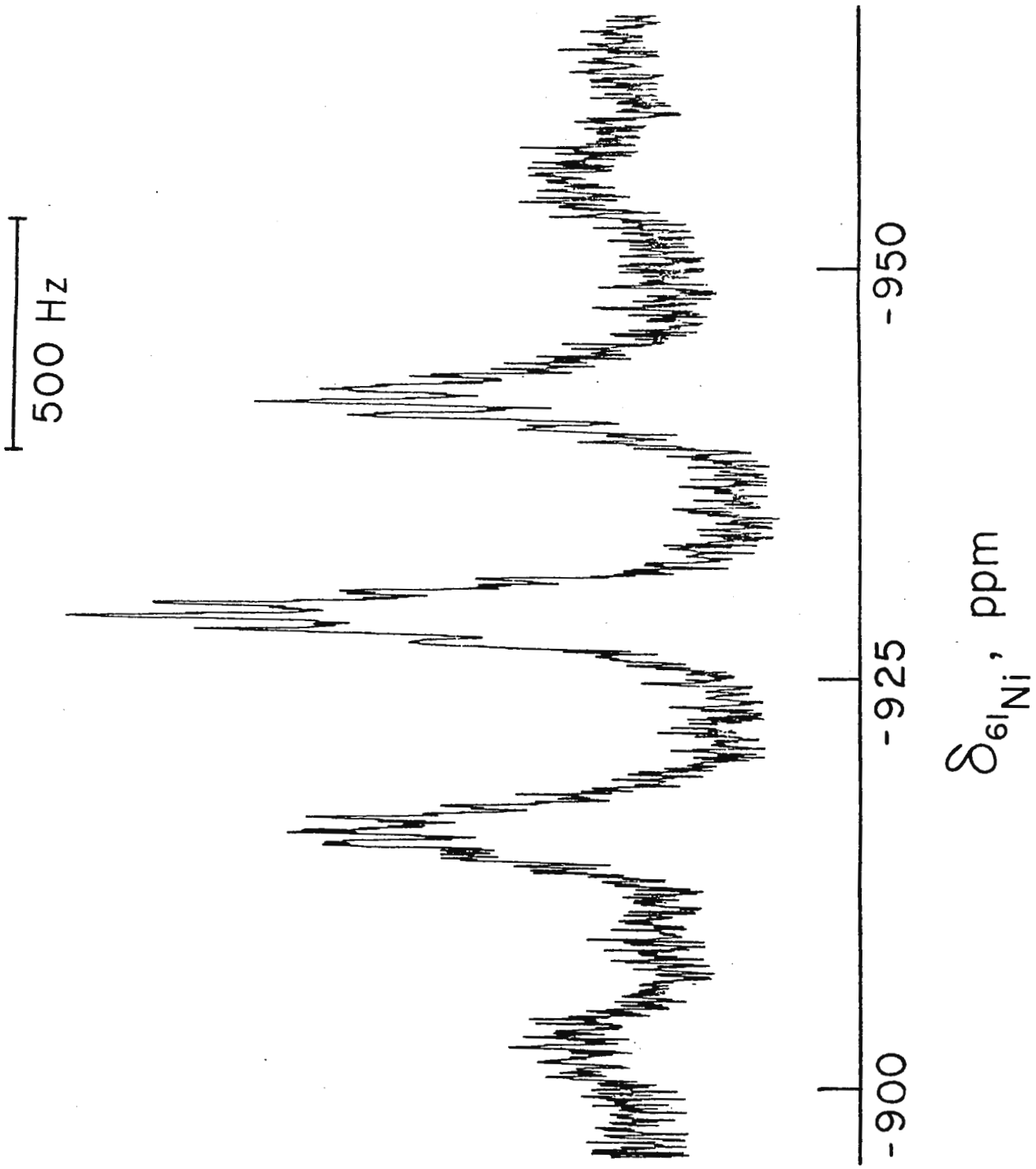
Figure 1 ^{61}Ni Spectrum of $Ni(PF_3)_4$ in THF



CHEMICAL CENTER
PHYSICAL CHEMISTRY 2

Lund, February 2, 1982

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

Title: Our new toy, a Nicolet 360.

Dear Barry,

In response to your reminder we have the following to report.

Firstly, we have recently acquired a Nicolet 360 WB spectrometer which is actually a 361.7 MHz machine. Of course for us, who have been used to work with the old-fashioned XL-100 or our home-built 6 Tesla spectrometer with a very simple program, the Nicolet software is just like a dream (or sometimes a nightmare). The spectrometer has mostly behaved quite well and as a simple example we want to show a few proton difference spectra from heart troponin C. The spectra are differences between samples containing various amounts of calcium ions as indicated in the Figure. The fact that the spectrum does not change to any significant degree between 3 and 4 equivalents of calcium is in agreement with other measurements showing that the heart troponin C does not bind more than 3 equivalents of calcium. Secondly, it might be of interest to other Nicolet owners that we have built our own low frequency probes for this spectrometer with horizontally arranged non-spinning samples. The resolution allowed by this probe is not overwhelming but as can be seen from Figure 2 it is more than adequate for our studies of quadrupolar ions like ^{39}K, ^{25}Mg or ^{43}Ca.

Sincerely,

Olle Teleman Torbjörn Drakenberg Sture Forsén

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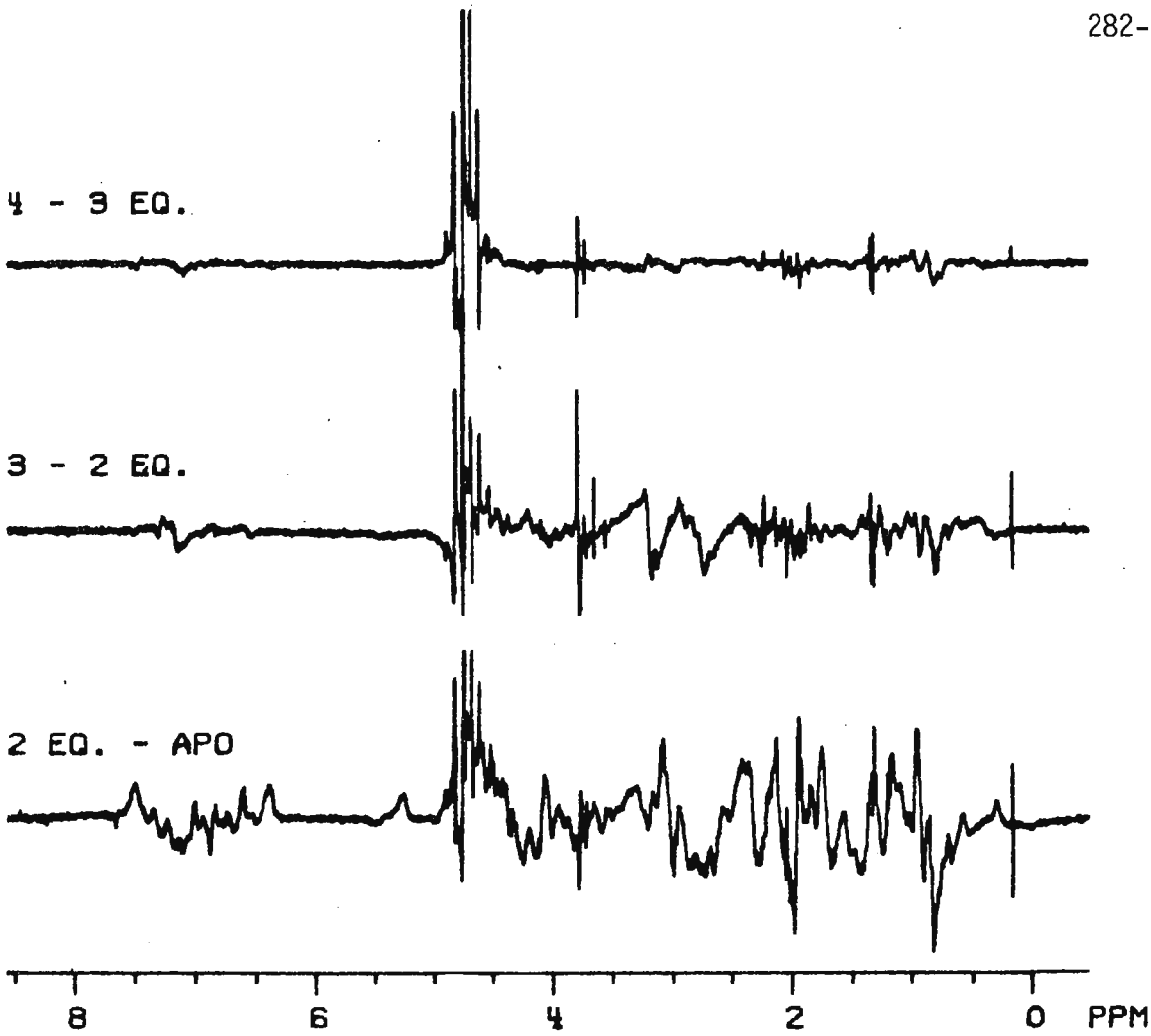
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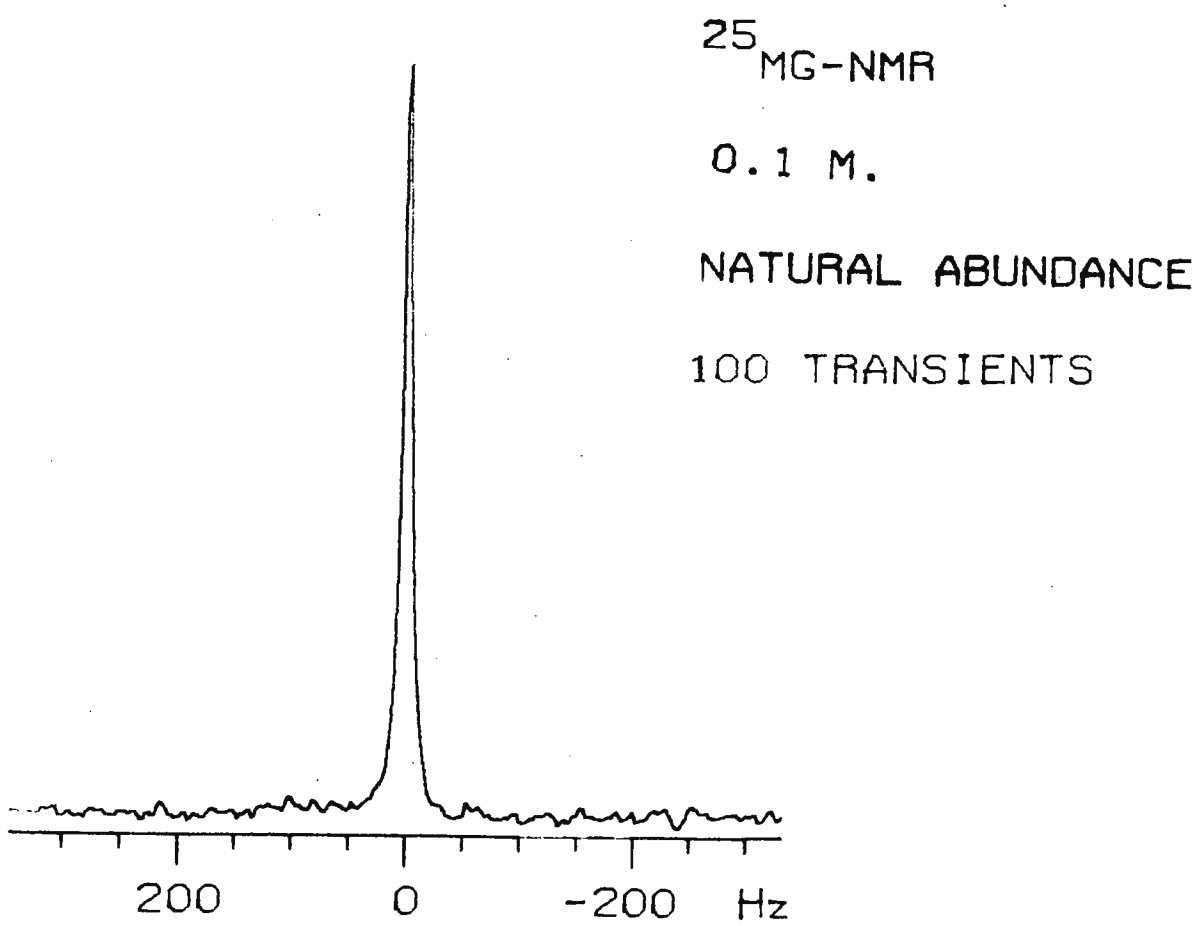
25 MG-NMR
0.1 M.
NATURAL ABUNDANCE
100 TRANSIENTS
200
0
-200
Hz

The University of Manitoba

Department of Chemistry
Winnipeg, Manitoba
Canada R3T 2N2

February 22, 1982

Dear Barry:

Oh Constancy, thy name is J! Inept INEPT!

In principle, the chemical shift is magnetic-field dependent (1,2), as is the atomic hyperfine constant(3). Although it is normally assumed that J is independent of the magnetic field, one might imagine a distortion of a molecule in a large magnetic field, causing a change in J; or, say, a partial alignment of the solvent or solute molecules(4) leading to an alteration of the solvent dependence of J.

Rudy Sabastian prepared a (degassed) ca/mol% solution of $CHCl_2F$ in C_6D_6 and a ca 11 mol% solution of 2,4,6-tribromoiodobenzene in C_6D_6. On one of his trips to Guelph, Rod Wasylishen measured $^2J(H,F)$ as 53.33 Hz in the first compound at 400MHz and $'J(H,^{13}C)$ as 175.11 Hz in the second. Kirk Marat found, at 90MHz, that these couplings are 53.33 and 175.11 Hz, respectively (same samples, of course). Perhaps one should try this experiment on a very large J... .

In another experiment at 23.63 MHz, Kirk Marat and Richard Veregin recorded the ^{13}C-4 triplet of 4-chloro-3,5-dinitrobenzotrifluoride: $J(H, ^{13}C)$ is ca 8Hz and we ignore coupling to ^{19}F. Weak and constant irradiation of one 'H peak yields what looks like an INEPT ^{13}C spectrum: the central peak vanishes,the outside peaks (one inverted) are up in intensity by a factor of ca5. As Ray Freeman once said, "people are tickling more and more and enjoying it less and less". Help!

Technically and otherwise yours,

Ted

Ted Schaefer.

TS/pp

1. N.F. Ramsey. Phys. Rev. A1, 1320(1970).

2. D.M. Doddrell, D.T. Pegg, and M.R. Bendall. Aust. J. Chem. 32, 1(1979).

3. N.P. Economou, S.J. Lipson, and D.J. Larson. Phys. Rev. Lett. 38, 1394 (1977).

4. T.M. Plantenga, H. Bulsink, C. MacLean, and J.A.B. Lohman. Chem. Phys. 61, 271 (1981).

THE ROCKEFELLER UNIVERSITY
1230 YORK AVENUE · NEW YORK, NEW YORK 10021
212-570-8270

16 February 1982

Professor R. B. Shapiro
TAMU Newsletter
Texas A & M University
College Station, Texas 77843

Dear Dr. Shapiro:

POSTDOCTORAL VACANCIES

I have two immediate vacancies at the postdoctoral level for recent graduates to work in physical biochemistry using NMR.

For one position, we wish to continue and extend our studies of dynamic conformations of peptide and small proteins using NMR and modified or isotopically substituted materials. Candidates with experience in peptide or protein chemistry will be particularly appropriate. The salary will be competitive, and appointment as a Research Associate is possible for exceptionally qualified candidates.

The second vacancy is for a postdoctoral fellow to investigate the effects of novel sterols on cholesterol/phospholipid systemsusing a variety of physical techniques, principally -- of course -- NMR. The salary is in the normal NIH postdoc range. There may be an opportunity for this project to develop along more physiological lines, if the results and the researcher so indicate. Since this position is part of a training grant from NIH, only US nationals or permanent residents are eligible, by Federal law.

Anyone interested in these positions should write to me and arrange for letters of recommendation to be sent.

Sincerely,

David Cowburn

DC:mmh

David Cowburn

CHEMICAL INSTITUTE

UNIVERSITY OF AARHUS

DEPARTMENT OF ORGANIC CHEMISTRY
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Telephone (06) 12 46 33

February 2, 1982
HJJ/ATL

Professor B.L.Shapiro
Department of Chemistry
Texas A & M University
COLLEGE STATION - Texas 77843
USA

Re: The Flip Angle Effect in the Determination of the Sign for $^{1}J(^{15}N-^{15}N)$ Using SPT

Dear Barry,

After working with supercooling of some aqueous solutions (TAMU NMR 277-47) (1) in hot South Carolina last summer, I am now back to normal temperatures in the cold winter of Scandinavia. Recently one of my students, Theo Berkhoudt, completed some nice ^{15}N NMR work on the determination of the sign of the one-bond $^{15}N-^{15}N$ coupling constant in ^{15}N doubly-enriched 1-phenylpyrazole, 1, using $^{15}N-\{^{1}H\}$ selective population transfer (SPT) (2). Although there has been quite some interests in semi-empirical calculations of $^{15}N-^{15}N$ coupling constants (3), we are aware of only one experimental report on the sign of such couplings. In nitrous oxide (N_2O) a negative sign is claimed for $^{1}J(^{15}N-^{15}N)$ (= -9.16 Hz) based on liquid crystal NMR techniques (4).

Whenever a nonselective "read" pulse is applied to homonuclear spin systems at nonequilibrium states, the so-called "flip angle effect" must be considered in order to interpret the intensities of the individual transitions. In the present $^{15}N-\{^{1}H\}$ SPT experiments for 1, nonequilibrium states are created by the ^{1}H SPT π-pulses. Thus, the flip angle effect becomes important for the determination of the relative signs of coupling constants as described recently (5). The accompanying figure depicts some $^{15}N2$ spectra with the SPT π-pulse applied at the two H3 transitions at highest frequency and using various flip angles for the ^{15}N "read" pulse. For a 90° flip angle (Figure c) no relative sign information for the $^{15}N-^{15}N$ cou-

pling constant is obtained (5). However, the spectra determined with flip angles of 60° (Figure b) and 120° (Figure d) show (5) that $^{1}K(^{15}N1-^{15}N2) \times {}^{3}K(^{15}N1-H3) < 0$ and $^{3}K(^{15}N2-H4) \times {}^{3}K(H3-H4) > 0$; therefore, $^{1}J(^{15}N-^{15}N) < 0$ (= -12.85 Hz), since $^{3}J(^{15}N1-H3) < 0$ is determined from other experiments. Preprints on a brief report of this work are available.

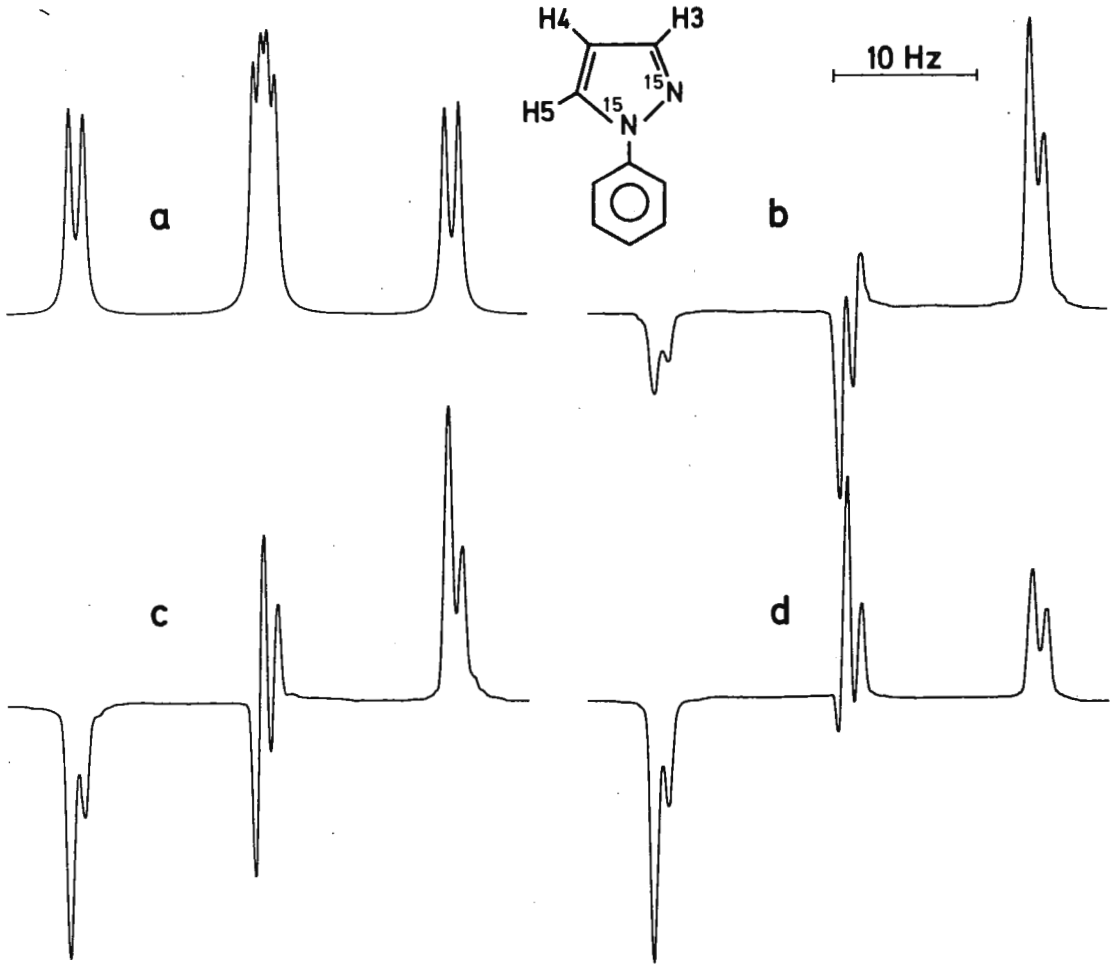


Figure. (a) Simulated proton coupled ^{15}N NMR spectrum for the $^{15}N2$ nitrogen in 1-phenyl-[$^{15}N_2$]-pyrazole. (b-d) Experimental $^{15}N2-\{H3\}$ SPT π-pulse spectra all obtained with the same π-pulse irradiation frequency (at the two H3 transitions at highest frequency) but with flip angles of 60° (figure b), 90° (figure c), and 120° (figure d) for the ^{15}N "read" pulse.

Sincerely,

Theo Berkhoudt Hans J. Jakobsen

(1) H.J.Jakobsen and P.D.Ellis, J.Phys.Chem. 85, 3367 (1981).
(2) H.J.Jakobsen and W.S.Brey, J.Am.Chem.Soc. 101, 774 (1979).
(3) Tun Khin and G.A.Webb, J.Magn.Reson. 33, 159 (1979) and refs. cited.
(4) P.K.Bhattacharyya and B.P.Daily, J.Chem.Phys. 59, 5820 (1973).
(5) O.W.Sørensen, H.Bildsøe, and H.J.Jakobsen, J.Magn.Reson. 45, 325 (1981).

DEPARTMENT OF BIOCHEMISTRY

THE UNIVERSITY OF ALBERTA
MEDICAL SCIENCES BUILDING
EDMONTON, CANADA T6G 2H7

PHONE: (403) 432-5460

February 5, 1982

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

Re: Low Concentrations by NMR

Dear Barry:

NMR methods are often criticized in comparison with other techniques used in biochemistry because of its low sensitivity. We feel (as do many others I'm sure) that this is a bit of a bum rap. We have been studying the occupancy by ytterium of the two metal binding sites on the calcium binding protein parvalbumin using ^{1}H NMR. The shifted resonances at 15.4 and 14.8 ppm are diagnostic for the two sites and there was some possibility that aggregation at high protein concentrations (1×10^{-3}M) was influencing the relative occupancies. In the enclosed figure we go down to 17×10^{-6}M with no change in relative intensities. The spectra were run on a Bruker HXS-270 spectrum; the 17 μM spectrum used a 10 mm tube, NA-360,000, TT=20.5 hrs.

These resonances are broad, but have correspondingly short T_1's. Floating point arithmetic was not necessary until we went to concentrations lower than 17 μM like 9 μM. The limiting factor in these studies is baseline distortions.

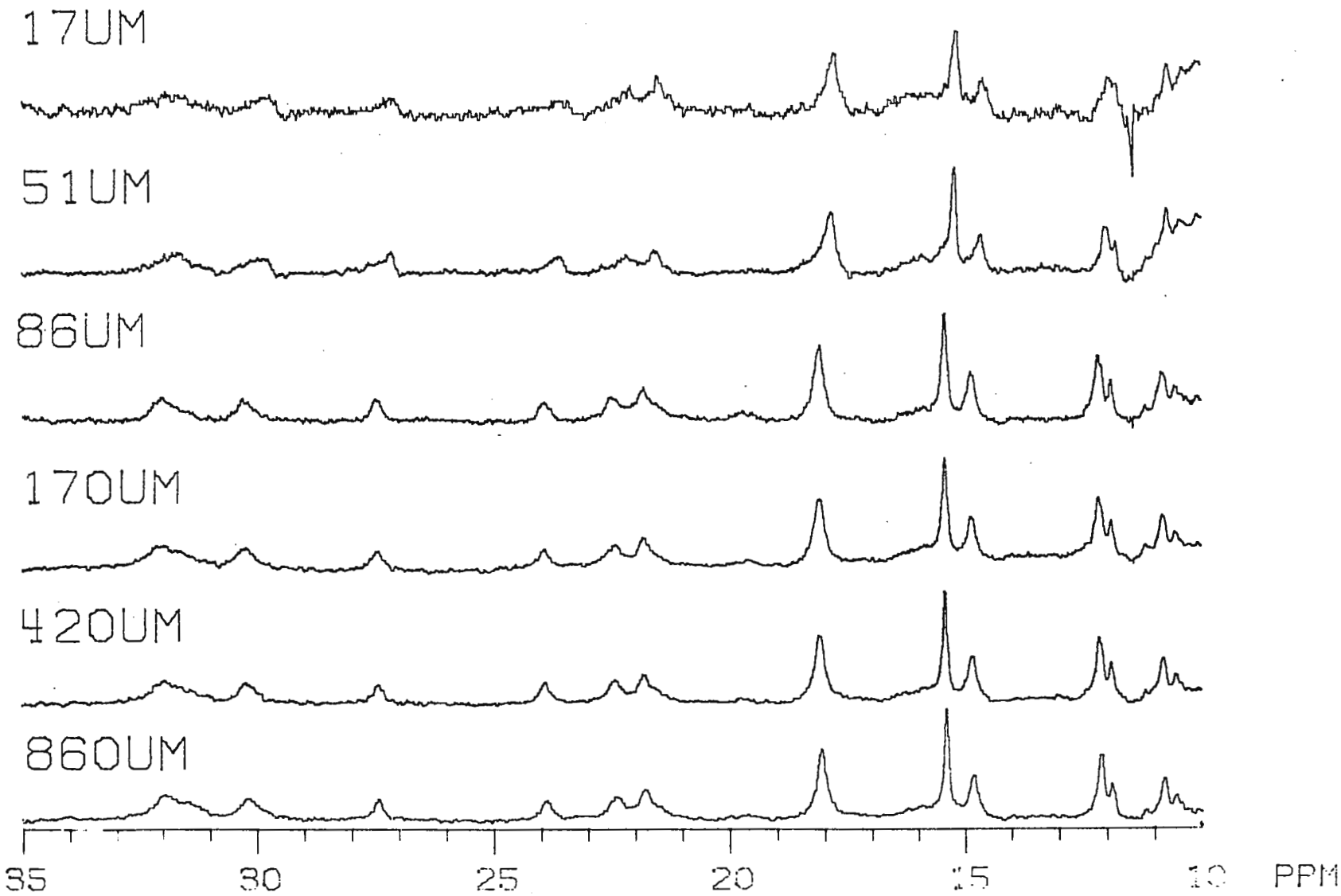
Best regards,

Gerard Brian

Lana Lee Gerard McQuaid Brian D. Sykes

/pm

Enclosure


17UM
51UM
86UM
170UM
420UM
860UM
35
30
25
20
15
10
PPM

282-23

TECHNISCHE HOGESCHOOL DELFT

Laboratorium voor Technische Natuurkunde

Bereikbaar met buslijn 60 en 63 (station N.S.-Delft)

Dr. Bernard L. Shapiro
Department of Chemistry
Texas A & M University
COLLEGE STATION TX 77843
U.S.A.

Uw kenmerk	Uw brief van	Ons kenmerk	Datum	Delft, Lorentzweg 1
		JS/MM/059	9 February 1982	Doorkiesnummer (015) 78

Onderwerp

A BOOK OF AD BAX ABOUT 2D-SPECTROSCOPY

Dear Professor Shapiro,

After having finished his studies in our group of magnetic resonance Ad Bax stayed some more years to work on his thesis about the above mentioned subject, which was ready in November 1981. A considerable part of his reasearch work was done with Dr. Freeman in Oxford.
As from various sides was insisted on publication in bookform of his thesis, he decided to do so. The book will be published under the title: "Two-dimensional nuclear magnetic resonance in liquids".
We believe that the book is the first to cover the field of two-dimensional nuclear magnetic resonance spectroscopy in liquids.
It gives an impression of the possibilities of two-dimensional spectroscopy and provides a practical guide for those who actually want to use the new techniques. The theory underlying the various methods is presented in a way that is easy to understand and requires only an elementary knowledge of conventional Fourier Transform spectroscopy.
The contents of the different chapters is:

1. General aspects of two-dimensional NMR spectroscopy
2. Chemical shift correlation spectroscopy
3. J-spectroscopy
4. Multiple quantum coherence
5. Carbon - carbon coupling observed in natural abundance samples

Algemeen telefoonnummer T.H. (015) 789111
Correspondentieadres: Postbus 5046, 2600 GA Delft

812340

LABORATORIUM VOOR
TECHNISCHE NATUURKUNDE
DER TECHNISCHE HOGESCHOOL DELFT

~~NEWSLETTER~~BLAD No.
BRIEF No. 059 d.d. 9 February 1982

6. Problems and methods

7. Spectrometer- and computer requirements

Moreover there are 3 appendices viz.:

Appendix I Example of a density matrix calculation
Appendix II Magnetization transfer in $^{13}CH_2$ and $^{13}CH_3$ groups
Appendix III The effect of a single selective pulse.

In the U.S.A. and Canada the book will be sold by

Kluwer Boston Inc.,
190 Old Derby Street
HINGHAM MA 02043
USA

and in all other countries by

Kluwer Academic Publishers Group
P.O. Box 322
3360 AH DORDRECHT
The Netherlands

The price of the book will be $ 29,50 and the ISBN number is 9027714126.

In Hingham the book will appear in the beginning of June and in Dordrecht one month earlier.

His promotors,

Dr.Ir. A.F. Mehlkopf

Prof.Dr.Ir. J. Smidt

282-25

Department of Chemistry
State University of New York at Stony Brook
Long Island, NY 11794
telephone: (516) 246-5050

StonyBrook

18 February 1982

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

"Post-doctoral Position Available"

Dear Barry:

A position is available in April 1982 to work on NMR and ESR studies of E. coli membrane proteins. The project is a collaborative one with Professor Masayori Inouye of the Department of Biochemistry, and involves isotopic, chemical and spin labelling as well as spectroscopic studies on solutions, membrane preparations, and intact bacteria. Interested candidates should contact me or Professor Inouye, submitting a curriculum vitae and arranging for two letters of recommendation.

The State University of New York at Stony Brook is an equal opportunity/affirmative action employer.

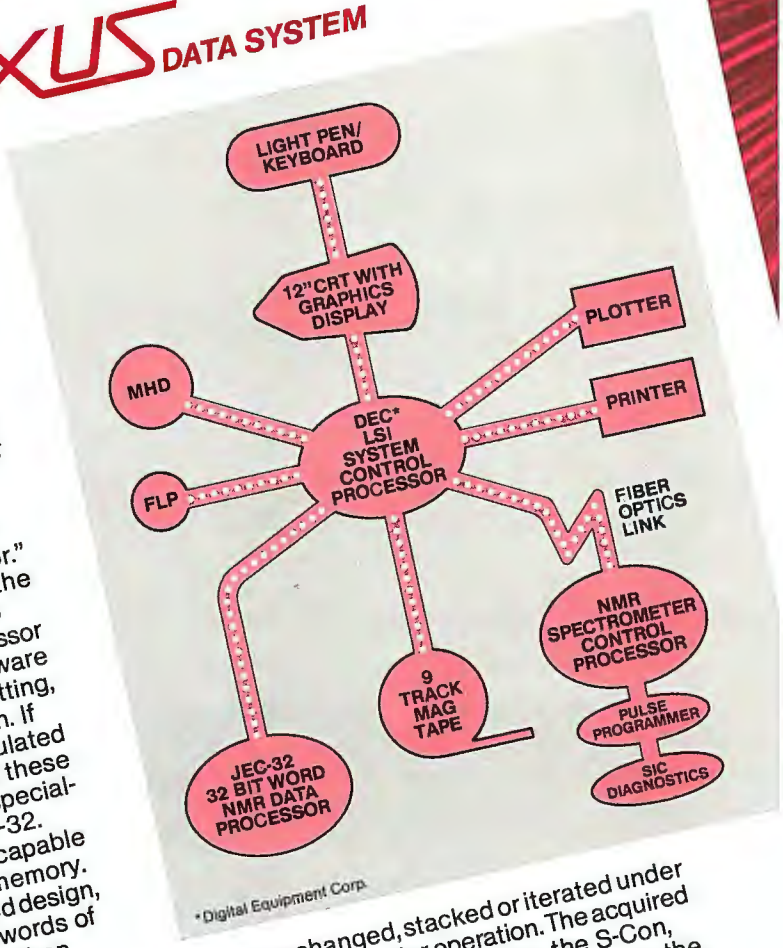
Yours truly,

Paul C. Lauterbur
Professor of Chemistry and
Research Professor of Radiology

PCL:eg

JEOL GX REPORT #1

THE plexus DATA SYSTEM



PLEXUS: An interwoven network of parts or elements in a system.

There is no better way to describe the data processing philosophy incorporated into the GX-400/500 FT-NMR spectrometers. To accommodate the increased demands placed on an FT-NMR data system, the PLEXUS data system deviates from the usual single computer approach. A multi-computer network using distributed processing software is employed to achieve trend setting levels of performance for speed, efficiency, and flexibility.

The center of the PLEXUS data system is the Digital LSI "system control processor." All interaction between the operator and the spectrometer pass through this hub. Job assignments are determined by this processor and distributed to the appropriate hardware for execution, for example; printing, plotting, disc storage or spectrometer operation. If actual data is to be acquired or manipulated (Fourier transformation, phasing, etc.) these jobs are assigned to a second, highly specialized "NMR data processor," the JEC-32.

The JEC-32 is a 32-bit computer, capable of accommodating 256K words of memory. Because of its unique and specialized design, fast Fourier transformations of 8K words of data (32 bit words) are done in less than 3 seconds! The real value of this amazingly fast FFT time can be appreciated more fully when considering large data sets, especially 2-dimensional FFT, where transform times are decreased dramatically, making 2-D NMR a much more practical and efficient experiment.

The spectrometer system is made complete by total computer control over all spectrometer functions by the PLEXUS data system. Through the "system control processor" and "spectrometer control processor," PLEXUS totally controls all spectrometer variables, including lock offset, lock phase, lock level, receiver gain and all irradiation and observation phases allowing any NMR parameter to be changed, stacked or iterated under unattended computer operation. The acquired experimental data is sent from the S-Con, over distortion-free fiber optics cables, to the JEC-32 where data treatment is carried out.

A further benefit of the PLEXUS concept is the SIC diagnostics (Status Integrity Check) which monitors all of the spectrometer hardware through status registers located on each board. Valuable service information concerning NMR hardware and computer components can then be extracted directly from the GX spectrometer or remotely.

For further information, call . . .

JEOL
235 Birchwood Ave., Cranford, NJ 07016
201—272-8820

JEOL (U.S.A.), INC. • ANALYTICAL INSTRUMENTS DIVISION
235 BIRCHWOOD AVENUE • CRANFORD, NEW JERSEY 07016
TELEX NO. 13-8840 • (201) 272-8820

February 25, 1982

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

Dear Barry:

We are currently looking for a chemist who understands instrumentation, such as NMR, and who cannot afford his own home computer to do all those "neat" things a chemist would like to do.

The position is a newly created one and would fall under the category of software R&D, with emphasis on development of the GX series system. Familiarity with a high level language such as FORTRAN or Pascal and a good knowledge of state of the art operating systems, preferably DEC, is necessary. Additional knowledge in graphics, data transfer, networking, and "friendly" software would be useful. Degree level is quite flexible since the unique mix of skills is more important.

Anyone interested should send a brief resume to Michael Albright at the above address.

Sincerely,

Michael J. Albright
NMR Product Manager

MJA/mjd

University of Bristol **School of Chemistry**

Cantock's Close
Bristol
England BS8 1TS

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

9th February, 1982

Dear Professor Shapiro,

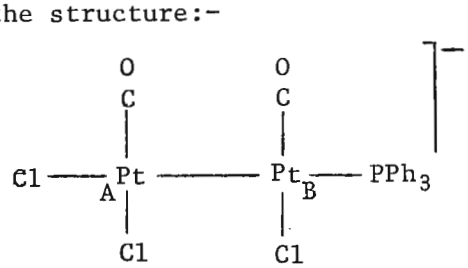
Applications of ^{195}Pt n.m.r.

We are very pleased with the performance of our JEOL FX90Q on ^{195}Pt which is fortunate since our chemical work centres on this element. Our maximum frequency range is 50k Hz but we usually use 40k Hz (just over 2 000 ppm). When necessary the range is increased by acquiring a set of spectra with automatically incremented observation frequencies. Using 8K points the acquisition time is ca. 0.12s or 30,000 pulses in an hour. Despite this rate, the relaxation of all but the most symmetric molecules is fast enough for 90° pulses to be used. We reference the spectra via the ^{2}D lock signal so that for our spectrometer $\Xi(^{195}Pt)$ = 21.4 MHz corresponds to 19.175 263 MHz for a ^{2}D frequency of 13.754 839 MHz set on CD_2Cl_2.

Of course, many spectra consist solely of singlets which may be confused with external interference etc. Much more interesting patterns arise when other spin-active nuclei are present and this can include ^{195}Pt in dimeric species. To evaluate $^{1}J(PtPt)$ in the symmetric dimers $[Pt_2X_4(CO)_2]^{2-}$ (X = Cl or Br) and $[Pt_2(C_5H_5)_2(CO)_2]$ we prepared samples with ca. 75 % ^{13}C enriched CO. We had to compromise between spectra broadened at room temperature because of CO exchange and broadening at low temperatures because of increased relaxation. The cyclopentadienyl complex gave the most detailed spectrum which is shown in Figure 1. The 'inner lines' (marked *) of the $[AX]_2$ spin system (^{13}C-^{195}Pt-^{195}Pt-^{13}C) give a value of 9 400 ± 70 Hz for $^{1}J(PtPt)$ and a further, less accurate value can be obtained from the [ABX] system (^{13}C-^{195}Pt-^{195}Pt- marked o). As can be seen there is a significant isotope shift (0.8 ppm to high frequency for ^{195}Pt bound to ^{12}C compared to ^{13}C). Figure 2 illustrates an easier way to get values of J(PtPt). Replacement of a chloride ligand on one end of $[Pt_2Cl_4(CO)_2]^{2-}$ by iodide renders the Pt nuclei inequivalent and an 'AB' pattern due to J(PtPt) results. (I am afraid that infrared was necessary to show that the heavier halide goes opposite the Pt-Pt bond).

In fact the observation of Pt-Pt coupling can be a useful aid when investigating the reactions of dimeric platinum complexes. Thus after reacting $[Pt_2Cl_4(CO)_2]^{2-}$ with one PPh_3 ligand, the ^{195}Pt spectrum shows two doublets with Pt-Pt coupling between them confirming the structure:-

$\delta(^{195}Pt)$	
A	800 ppm
B	347 ppm



$^{1}J(PtPt)$	1 914 Hz
$^{1}J(PtP)$	2 334 Hz
$^{2}J(PtP)$	1 123 Hz

Yours sincerely,

R. J. Goodfellow I. R. Herbert

R. J. Goodfellow I. R. Herbert

Figure 1. ^{195}Pt n.m.r. spectrum of $Pt_2(C_5H_5)_2(CO)_2$ at -80 ^0C.

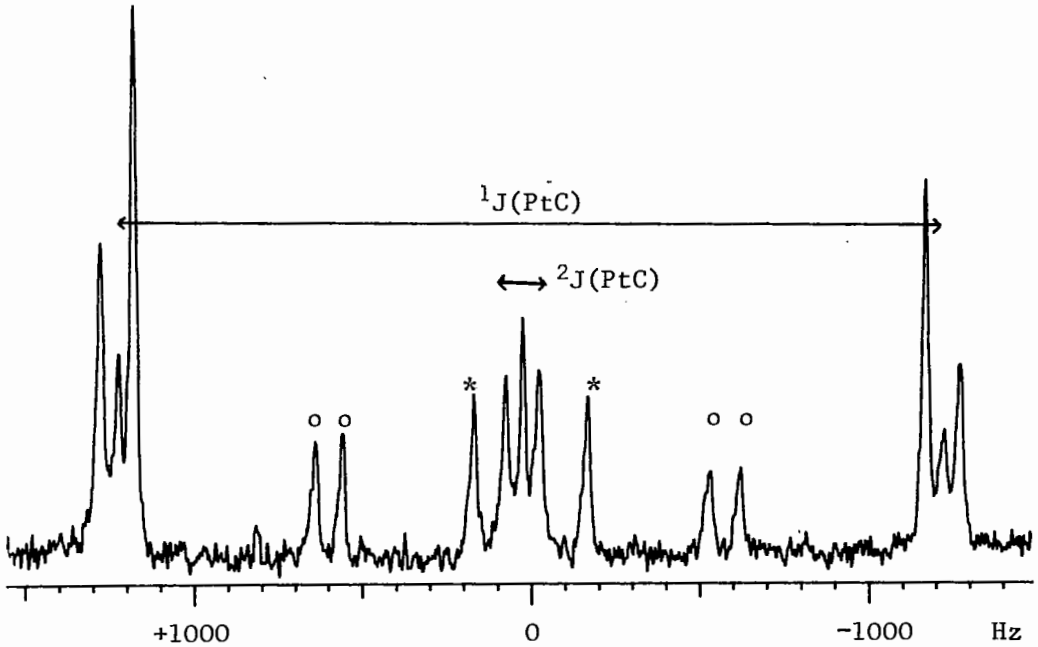
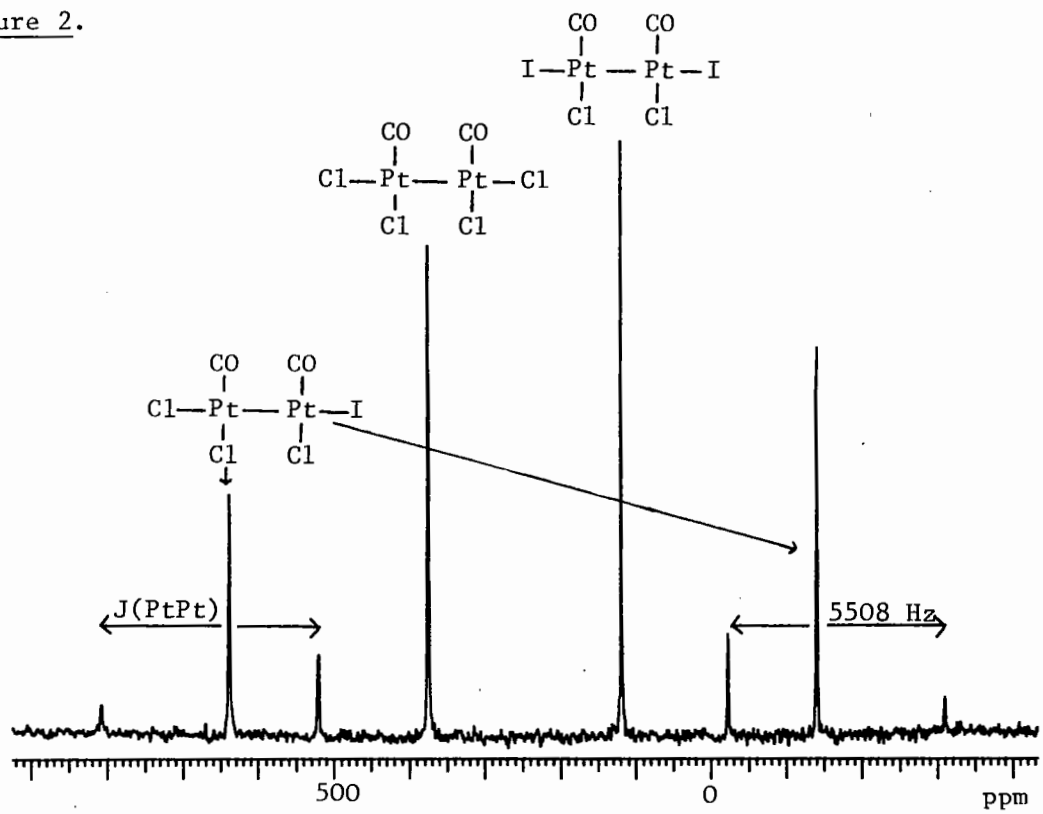


Figure 2.



BRUKER Instruments, Inc.
MANNING PARK
BILLERICA, MASSACHUSETTS 01821
(617) 667-9580

February 12, 1982

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

"Computer Determination of Signal - to -Noise"

Dear Dr. Shapiro:

Before the widespread availability of computers, the only means of determining the signal-to-noise ratio of NMR data was by graphical methods. The following equation has been the standard way of measuring S/N from a plot of the data.

$$\text{Graphical } S/N = (S/N_{pp}) * 2.5$$

where S - peak intensity
N_{pp} - the peak-to-peak amplitude of a chosen segment of the baseline noise
2.5 - factor by which N_{pp} is divided to approximate RMS noise.

The S/N values determined in the above manner have a high degree of uncertainty due to both subjective [1] and statistical[2] factors. Computer calculated values are inherently more precise in that the root-mean-square noise is calculated directly from the digitized data.

$$\text{RMS noise} = \frac{(\Sigma \delta_i^2)^{\frac{1}{2}}}{n-1}$$

where n - number of data points
δ_i - deviation of the baseline point from zero.

However, the problem is that the RMS S/N value is approximately twice the graphically determined value for the same spectrum. This difference stems from the fact that for FT NMR, in which the noise distribution is Gaussian[3], the peak-to-peak noise is roughly 5 times the RMS noise.[4]

The 2.5 factor is appropriate for a Rayleigh distribution which is more descriptive of noise generated by a CW spectrometer.[3]

As a result, it seems to us that S/N values reported in the literature should also state how those values were determined in order to remove all ambiguity.

In our DISNMR program, the RMS S/N value is divided by two. The printout states this explicitly.

RMS (S/N) *.5 =

Sincerely,

Harold Boll

Harold Boll, Ph.D.
Software Department

James W. Cooper, Ph.D.
Vice President
Software Development

HB/c

1. D. Zeissow, "Online Rechner in der Chemie", de Gruyter, Berlin, 1973

2. S. Sykora and J. Vogt, Bruker Report; February 1979

3. R.E. Santini and G.W. Kramer "Errors Associated with S/N Measurement in NMR Systems" Paper presented to ASTM Subcommittee on NMR Standards, Asilomar, CA; February 21, 1979

4. ASTM Standard E367-76 (NMR), section 7, Note 2

STANFORD UNIVERSITY
STANFORD, CALIFORNIA 94305

STANFORD MAGNETIC RESONANCE LABORATORY

(415) 497-4062
(415) 497-6153

February 16, 1982

Dr. Barry L. Shapiro
Department of Chemistry
Texas A & M University
College Station, Texas 77483

HELICAL METHIONINE OLIGOPEPTIDES

Dear Professor Shapiro,

Thank you for the yellow note. We hope this contribution keeps the beloved TAMU coming.

Trifluoroethanol (TFE) has been shown by circular dichroism (CD) to be a helix-supporting medium for oligopeptides (1,2). It has been one of our interests to substantiate these CD studies using NMR techniques. We have previously discussed NMR studies for the methionine oligomer series, t-Boc-(L-Met)$_n$-OMe (3). Blocked homo-oligopeptide esters however present serious solubility and aggregation problems (4). This has led to the attachment of oligomers to macromolecular, solubilizing polyethylene glycols (PEG) in the liquid phase method of peptide synthesis (5).

Fig. 1 shows the backbone NH resonances for a blocked methionine oligomer series attached to PEG — t-Boc-(L-Met)$_n$-NH-PEG. These spectra were obtained despite three strong proton lines - two from solvent TFE and one from PEG ($\bar{M}_r$ 6,000). Six nonequivalent NH resonances are seen for the pentamer and seven for the hexamer. Increase of chain length from 6 to 7 was shown by CD to result in a transition from a disordered to a helical structure (2). By NMR this transition leads to a 1:1:3:1:1:1 envelope. Further elongation of chain length to the octamer gives a 2:1:2:1:1:1:1 envelope.

The singly resolved NH resonances of the PEG-bound pentamer and hexamer shift monotonically upfield with temperature (Fig. 2). However, at the heptamer and octamer, two NH resonances are seen to show little shift changes over the same temperature range. In fact, the temperature coefficients for these two NH resonances are 3-10 times lower than those reported for the intramolecularly hydrogen-bonded NH resonances of the cyclic alumichrome and gramicidin peptides (6,7). To my knowledge, they are the lowest NH temperature coefficients yet noted for a linear peptide in TFE.

Sincerely yours,

Anthony Ribeiro

Anthony Ribeiro

1. Becker, J. M. and Naider, F. (1974) Biopolymers 13 1747-1750.
2. Toniolo, C. et al. (1979) Macromolecules 12 620-625.
3. Naider, F. et al. (1980) Biopolymers 19 1791-1799.
4. Ribeiro, A. et al. (1979) Int. J. Pept. Prot. Res. 14 414-436.
5. Pillai, V. N. R. and Mutter, M. (1981) Acc. Chem. Res. 14 122-180.
6. Llinas, M. and Klein, M. (1975) J. Amer. Chem. Soc. 97 4731-4737.
7. Kumar N. G. et al. (1975) Biochemistry 14 2179-2207.

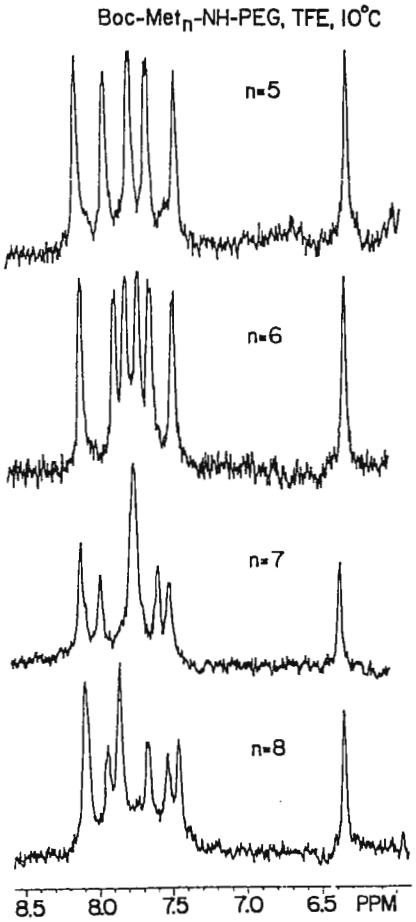


Fig. 1

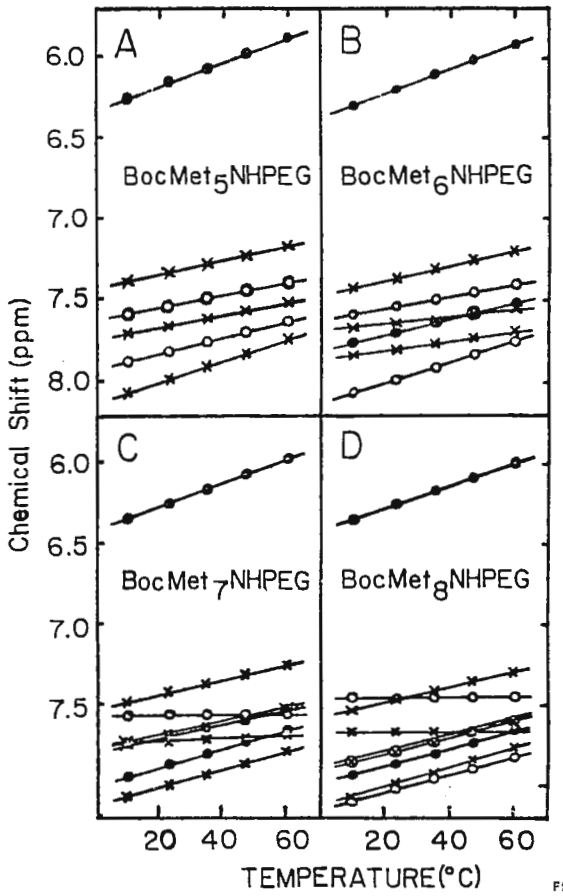


Fig. 2

Chemistry Department
The Open University,
Walton Hall,
Milton Keynes,
MK7 6AA.

Telephone Milton Keynes 74066 (Switchboard)
Milton Keynes 653606 (Direct Line)

THE OPEN UNIVERSITY

16 February 1982

To fellow-readers in the UK or elsewhere: I should be grateful to hear from anyone who has a V4331A or similar probe and inserts for a Varian 4300B wideline NMR spectrometer.

Thank you!

Joan Mason

Dr. Joan Mason

282-35

HARVARD MEDICAL SCHOOL

JEAN L. DELAYRE, Ph.D.
Research Associate in Biophysics

25 Shattuck Street
Boston, Massachusetts 02115
617 · 732-

February 18, 1982

Professor B. L. Shapiro
Department of Chemistry
Texas A-M University
COLLEGE STATION, TX 77843

MULTI-NUCLEI SURFACE COIL AT 8.2 TESLA

Dear Barry,

The use of Wide-Bore superconducting magnets has allowed people to look at larger samples, and it is now a current practice to study the metabolic activity of perfused organs in a 20mm or 30mm sample tube. If one wants to look at an organ (heart, brain, etc.) in an intact animal, one has to switch to the so-called surface coil to maintain a good sensitivity as well as a good spatial resolution.
In order for our Nicolet 360 Wide Bore NMR spectrometer to use this approach, , we have designed a special probe stack which can accomodate a whole rat and a movable broadband surface coil. In this configuration, one can easily observe different organs and position the surface coil very accurately (this is especially important for the heart). The design of the surface coil is such that it can be tuned at different frequencies (from 90 MHz to 160 MHz), thus allowing the observation of various nuclei such as sodium and phosphorus.

The two spectra shown here are representative of the kind of results we get : the first one is a phosphorus spectrum of a rat brain obtained in 200 seconds, without using any deconvolution technique; the second one represents the sodium spectrum of the heart of the same animal. Although it shows only one peak, it is very useful for positioning the coil close to the heart and for shimming purposes (one scan is enough to get a signal and shim on it). For more results, look for the poster of R. Graff which will be presented at the coming ENC (if accepted).

Yours sincerely,

Jean L. Delayre

RAT
BRAIN
P31

ONE-PULSE SEQUENCE

P2= 20.00 USEC
A DE= 125 USEC
D2= AT
D5= 1.00 SEC

NS = 200
SIZE = 2048
AT = 128.13 MSEC
ABC ON QPD ON = 1
ADC= 12 BITS AI= -1
SW= +/- 4000.00 DW= 125
F2= 360.068002
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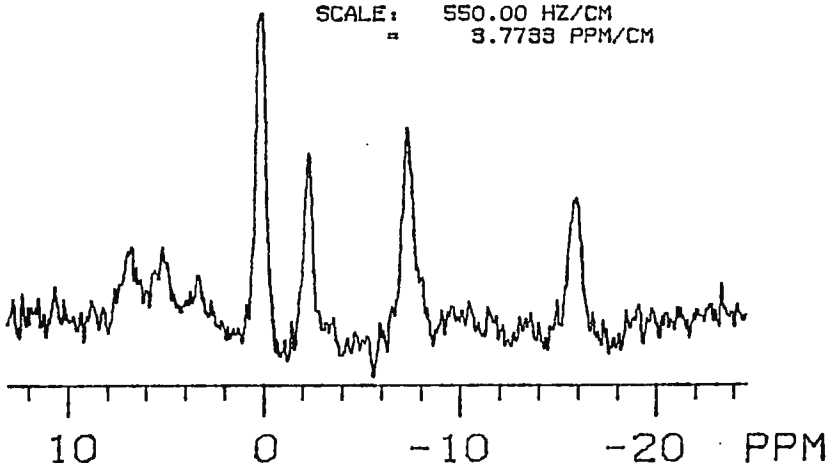

RAT
HEART
NA-23

ONE-PULSE SEQUENCE

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D2= AT
D5= 200.00 MSEC

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AT = 128.13 MSEC
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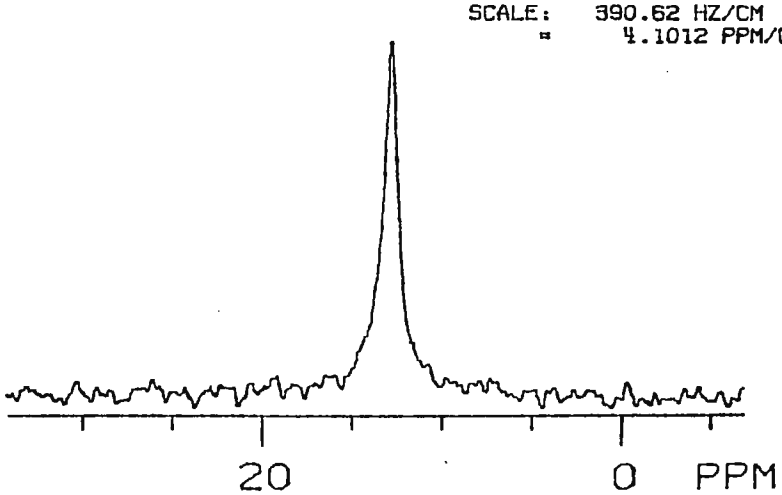

282-37

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- 5m and 10m ^{1}H variable-temperature probes
- ^{1}H and ^{2}H Internal lock channels
- B-SV3 PMX Pulse Amplifier
- B-S43 Bx Decoupler unit, with ^{1}H homonuclear decoupling channel
- Variable temperature control unit, -80 to +150°C
- Nicolet Mod. 180 Minicomputer with 80K word memory
- Diablo Mod. 33 Disk Drive, High Density (1.1 M words/disk)
- ASR-33 Teletype terminal
- Tektronix 602 Display unit
- Complete manuals, schematics, software
- Spectrometer has CW capability (long unused, but intact)

Please contact: Dr. Richard S. Hanson
Gray Freshwater Biological Institute
University of Minnesota
P.O. Box 100, County Roads 15 and 19
Navarre, MN 55392
(612) 471-8476

(Personnel Req. #2240)

NMR SPECTROSCOPIST to assist in the operation and maintenance of the NMR laboratory at the NCI-Frederick Cancer Research Facility. The laboratory is equipped with R12B, XL-100 and NT-300 NMR spectrometers. Routine maintenance and operation of the XL-100 spectrometer are the primary responsibilities for this position. In addition, opportunities for involvement in collaborative projects will be encouraged. A background in electronics and NMR spectroscopy with a MS or Ph.D. in an appropriate field preferred. Inquiries, resumes and references should be sent directly to:

NCI-Frederick Cancer Research Facility
Personnel Department
(Attn: Ms. Sharon Bushwaller, Req. #2240)
P. O. Box B
Frederick, MD 21701
(USA)

Inquiries may also be answered by Bruce D. Hilton, Ph.D., (301-663-2350)

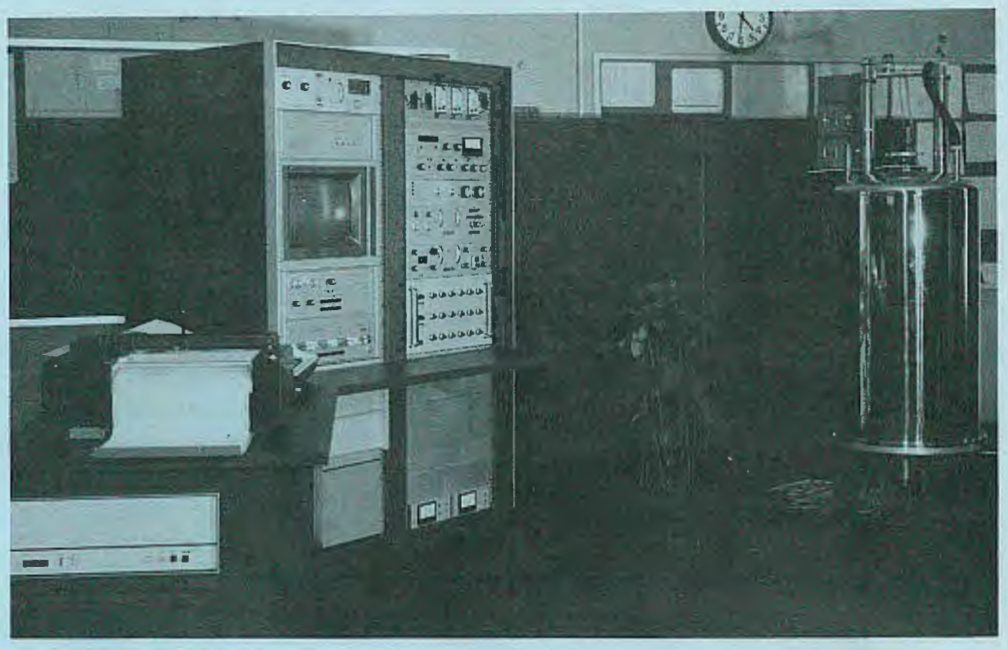
Nicolet Supercon FT-NMR Spectrometers

Uncompromising performance, limitless adaptability.

Our spectrometer systems have been conceived and designed to provide optimum performance while being fully adaptable to new techniques with minimal cost and difficulty. More than just a collection of instruments, they represent a completely modular approach to FT-NMR instrumentation that allows the user to expand his system as his research needs grow and to easily accommodate new experimental techniques as they develop.

Outstanding Nicolet features include these:

- **A full range of superconducting magnets from 4.7T to 11.7T (200MHz to 500MHz proton frequency range), in both wide-bore and narrow-bore configurations.**
- **Multinuclear observation with a wide variety of fixed-tune and broadband probes.**
- **Simultaneous acquisition, processing, and plotting for greater sample throughput.**
- **Simplified control of spectrometer operations and parameters by using easy keyboard commands.**



- **Advanced Nicolet 1180E Data System with 128K/20-bit memory, 256-step pulse programmer, and the most comprehensive FT-NMR software package available.**
- **Extended dynamic range performance with 40-bit acquisition and floating-point processing.**
- **An expandable pulse-sequence library, including T_1, T_2, Redfield, INEPT, homo- and hetero- 2D-FT, etc.**
- **Convenient computer control of field shimming, observe and decoupling frequencies, sample temperature, and probe-tuning.**
- **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:

- **High resolution studies of solids with Waugh-Pines cross-polarization and magic-angle spinning.**
- **High sensitivity wide-bore ^{13}C studies of high molecular weight polymers.**
- **Automated T_1 and T_2 measurements.**
- **Chemical dynamics studies.**
- **Temperature-programmed experiments.**
- **^{31}P experiments on living organs.**

NICOLET MAGNETICS CORPORATION
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THE SOLID LEADER in NMR

With Multi-Nuclear/ Multi-Field Solid State Probes

- **High field** solid sample probe for JEOL's 200 MHz SCM!
- ***Tunable heads** — interchangeable plug-in matching units for observation of
  - ^{13}C (~50 MHz)
  - ^{31}P (~80 MHz)
  - ^{29}Si (~40 MHz)

  with one probe!
- Self starting rotor/stator design!
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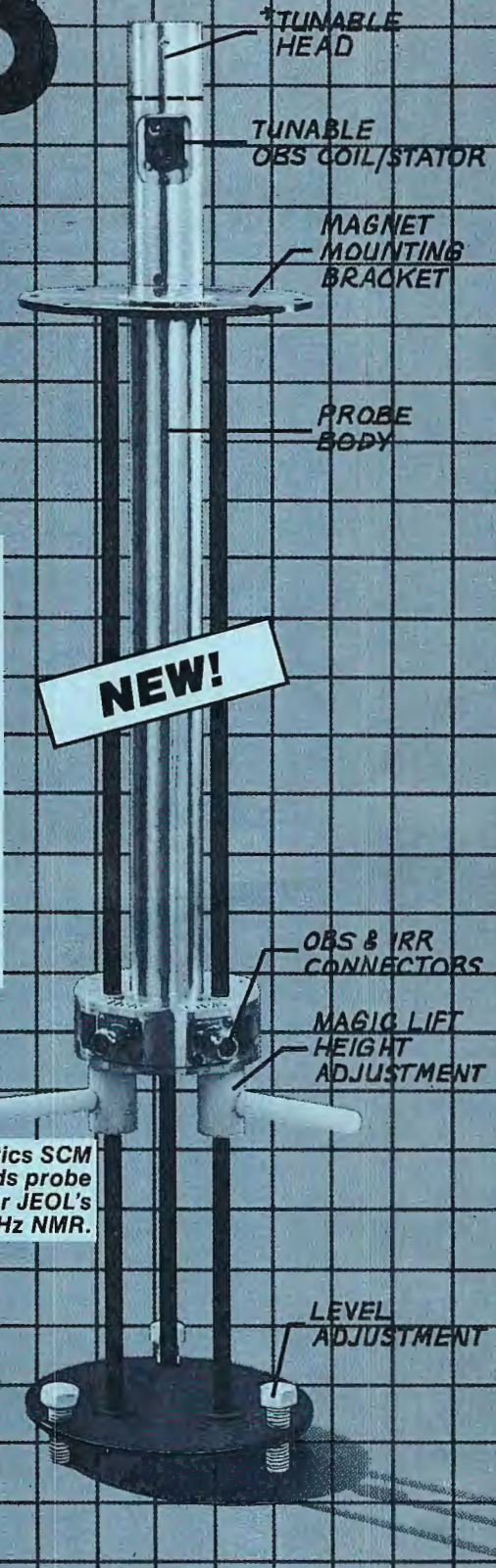
- **"Magic lift probe"** for quick sample change and probe insertion!
- All this, in addition to a full line of dual and broad-band high resolution liquid sample probes!



Chemagnetics SCM Solids probe for JEOL's 200 MHz NMR.

SOLIDS UPDATE – NOW AVAILABLE

- MULTI NUCLEAR SOLIDS PROBE FOR THE FX 270
- WIDE BORE MAGNET WITH VARIABLE TEMPERATURE SOLIDS FOR THE FX 200

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