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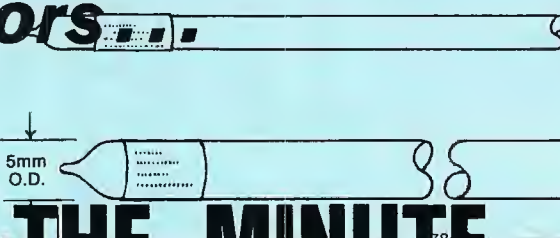
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DEADLINE DATES:	No. 293	7 February 1983
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All Newsletter Correspondence, Etc., Should be Addressed To:

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

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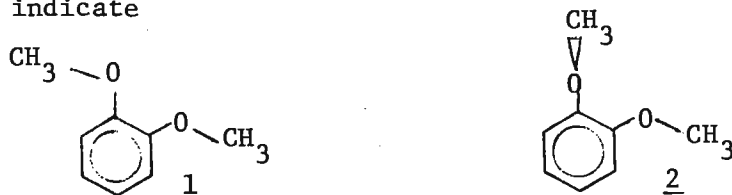
Nov. 22, 1982.

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

Dear Barry:

Conformational Behaviour of  $\text{OCH}_3$  and  $\text{SCH}_3$ .

Reino Laatikainen and Tim Wildman and I found it interesting that, for the gas phase, STO 3G calculations and a variety of experimental data strongly indicate



the "perpendicular" conformer 2 as more stable than the "planar" 1 (J. Am. Chem. Soc. 101, 2344 (1979)). Yet  $^{13}\text{C}$  shifts and some  $T_1$  measurements, e.g. in J. Med. Chem. 24, 906 (1981), imply that in solution the relatives of 1 are very likely stable. Now,  $^5J_{\text{O}^{\text{H}},\text{CH}_3}$  in anisole and its derivatives is negative (Tetrahedron Lett. 1999 (1969)) and is very likely a proximate coupling. As such, its magnitude (Tetrahedron 25, 877 (1969)) may well indicate the degree of nonplanarity of the  $\text{OCH}_3$  group.

Reino set out to analyze the 10-spin proton spectrum at 100 MHz of 1,2-dimethoxybenzene. After a herculean effort, employing NUMARIT (a program whose eventual appearance probably owes most to John Martin), he found  $^5J_{\text{O}^{\text{H}},\text{CH}_3}$  as  $-0.28$  (1) Hz; a value very close to that measured for anisole derivatives in which the  $\text{OCH}_3$  is pretty well forced to lie in plane (by the way, pretty well all the spins in 1 are coupled to each other).

So far so good. Reino then played the INDO FPT game as modified by Barfield (set certain Fock matrix elements to zero, thereby preventing "overlap" and the transmission of spin state information via various "paths"), with the results summarized in the attached figure. Two main points are of interest here:  $^5J_{\text{O}^{\text{H}},\text{CH}_3}$  is dominated by interactions via the methyl carbon orbitals and it drops off very rapidly (solid lines) as the  $\text{OCH}_3$  group twists out of plane. The diagram also suggests

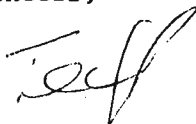
...cont'd...

Nov. 22, 1982,  
Prof. B. L. Shapiro,

that in anisole itself  $^5J_{H,CH_3}$  should lie near -0.13 Hz. Tim did a very careful analysis (not easy: you need very precise peak positions because  $\delta_O$  and  $\delta_P$  are so close) and found -0.14(1) Hz.

We therefore prefer to think that 1 is pretty stable in solution, compared to 2, and that anisole has a substantial barrier to rotation about the  $Csp^2-O$  bond, again in solution. Naturally, it makes sense to measure  $^6J_{P,H,OCH_3}$  in anisole and its derivatives. Reino and Tim have shown (INEPT comes in very useful as set up by Kirk Marat) that this  $^{13}C, ^1H$  coupling is  $\sigma-\pi$  dominated (just like  $^6J_{H,H}$ , see Acc. Chem. Res. 13, 400 (1980)). So we're off to the races, but may break a leg. Anybody have a 200 or 250 they would like to see the back of?

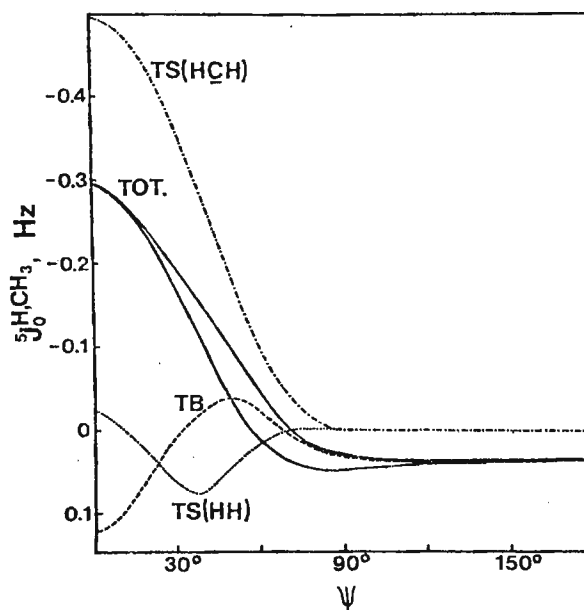
Cheers,



Ted Schaefer,  
Professor of Chemistry.

TS:dmp

P.S.:  $SCH_3$  behaves similarly to  $OCH_3$  with, of course, a lower barrier to internal rotation. You can make it sit perpendicular to the benzene plane by means of an internal hydrogen bond (Can. J. Chem. 60, 342 (1982)). This happens because, unlike oxygen, sulfur has a large 3p handle available for twisting. Small fingers are necessary and sufficient (rub them 100 times on cat's fur so as to give them a positive charge near the nail end).



**CHEMICAL CENTER**

PHYSICAL CHEMISTRY 2

Lund, November 22, 1982

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

$^{31}\text{P}$ -NMR in vivo measurements of smooth muscle metabolism

Dear Barry,

High resolution  $^{31}\text{P}$ -NMR studies of perfused skeletal muscle systems have been reported by many laboratories. We have embarked on the study of smooth muscle which has several physiologically and bio-chemically distinct properties. Utilising our homebuilt NMR spectrometer operating at 103 MHz equipped with a horizontal probe (5 or 10 mm), in which the muscles were isometrically mounted and superfused with oxygenated Tris buffer physiological saline solution (pH 7.4), (23°C), we have studied tissues obtained from rabbit urinary bladder, rabbit portal vein and rabbit and guinea pig taenia coli. Amounts of available tissue varied between 50 and 800 mg, requiring 4 hours and 10 minutes of spectral accumulation, respectively. The resonances observed in all spectra correspond to phosphocreatine (PCr) and ATP, the PCr to nucleotide ratio (varying between 1.5 and 2) was much less than observed for skeletal muscle but consistent with chemical determinations on tissue extracts. High levels of phosphomonoesters and inorganic phosphate were normally observed only in less viable preparations. Contraction in high  $\text{K}^+$  medium resulted in a small decrease in PCr, but did not alter ATP levels. Also addition of NaCN (1 - 2 mM) reversibly reduced the phosphocreatine levels, and caused only small changes in ATP levels. None of the above changes resulted in drastic alterations in intracellular pH, which was estimated to be 7.0. The intracellular  $\text{Mg}^{2+}$ /ATP ratio of about 1.5, and did not change upon perfusion with high  $[\text{Mg}^{2+}]$ , high osmolarity, or EDTA containing  $\text{Mg}^{2+}$ -free media. These results show that  $^{31}\text{P}$ -NMR can be fruitfully applied to the study of smooth muscle, although it has lower levels of phosphorylated metabolites than skeletal muscle tissues.

Sincerely yours,



Hans Vogel



Per Hellstrand



Sture Forsén

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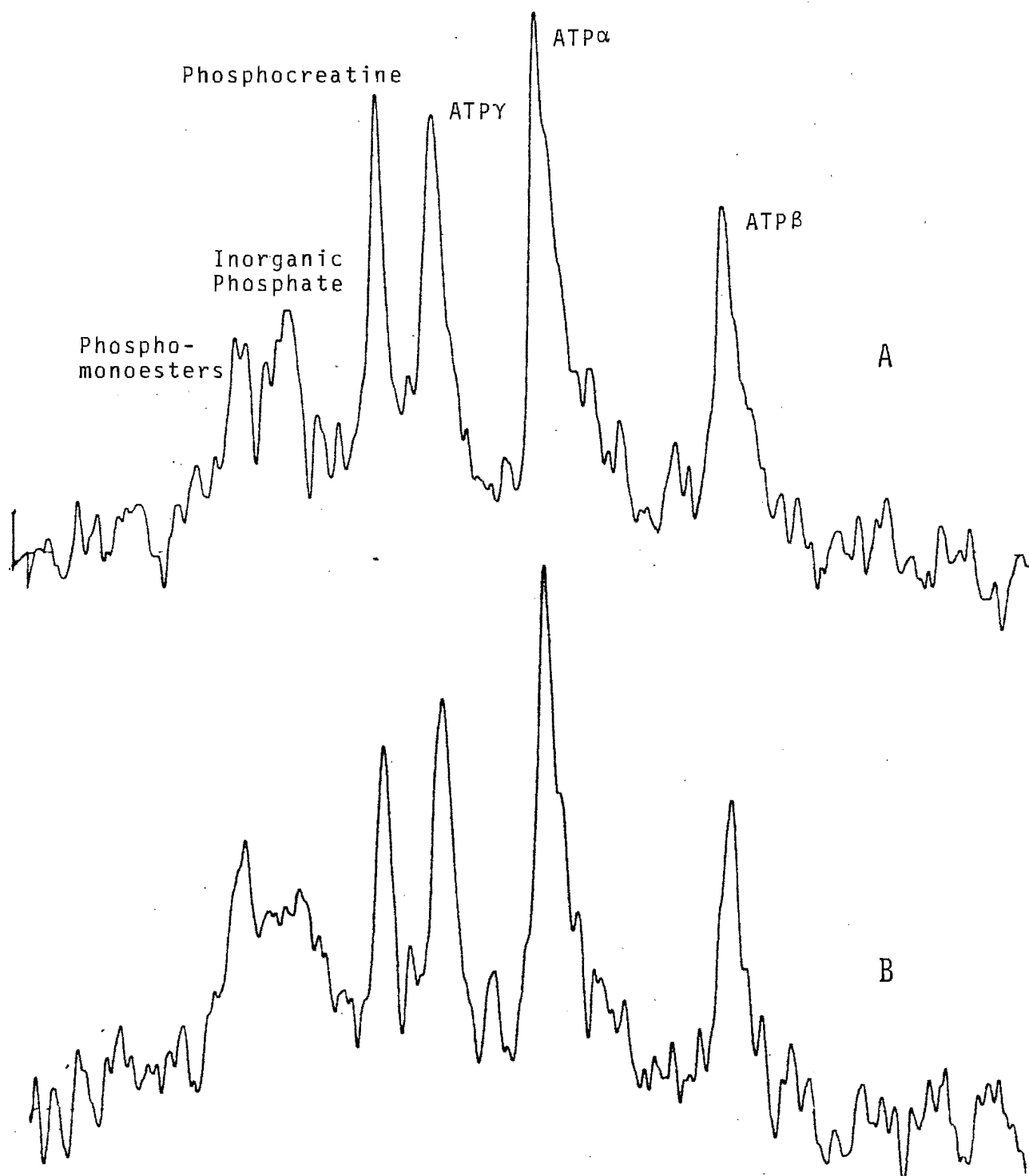


Fig 1.1 103 MHz  $^{31}\text{P}$ -NMR spectrum of rabbit urinary bladder (approx. 500 mg). A) resting, B) contracted with high  $\text{K}^+$  buffer. Note that the only difference between the spectra is the small decrease in the phosphocreatine resonance. Spectra were obtained in a 10 mm horizontal probe, a recycle time of 1 sec and a  $45^\circ$  pulse angle (25  $\mu\text{secs}$ ) with 2400 acquisitions for both spectra.



McMASTER UNIVERSITY  
Department of Chemistry

1280 Main Street West, Hamilton, Ontario, L8S 4M1  
Telephone: 525-9140

November 26, 1982

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

Dear Dr. Shapiro

<sup>209</sup>Bi NMR Spectrum of the Hexafluorobismuthate (V) ion.

Bismuth-209 is among the more sensitive nuclei, possessing a sensitivity relative to the proton of 0.137, but due to quadrupolar relaxation effects, the only solution studies of a <sup>209</sup>Bi resonance reported have been of aqueous solutions of Bi(NO<sub>3</sub>)<sub>3</sub> which gave broad resonances.

The compound (CH<sub>3</sub>)<sub>4</sub>N<sup>+</sup>BiF<sub>6</sub><sup>-</sup> was chosen for the present study and acetone was used as solvent. An acceptable <sup>209</sup>Bi spectrum obtained from a single transient on a Bruker WM250 consisted of a 1:6:15:20:15:6:1 septet. The <sup>19</sup>F spectrum recorded on a Bruker WH-90 consisted of an equal-intensity decet centred at -42.6 ppm with respect to CFC1<sub>3</sub>. The observed <sup>209</sup>Bi-<sup>19</sup>F coupling constant was 3323 ± 3 Hz in contrast to the solid state value (2700 Hz) estimated previously<sup>2</sup>.

A fuller account will appear in the Journal of Magnetic Resonance, February, 1983.

Sincerely

Keith Morgan

Brian G. Sayer

Gary J. Schrobilgen

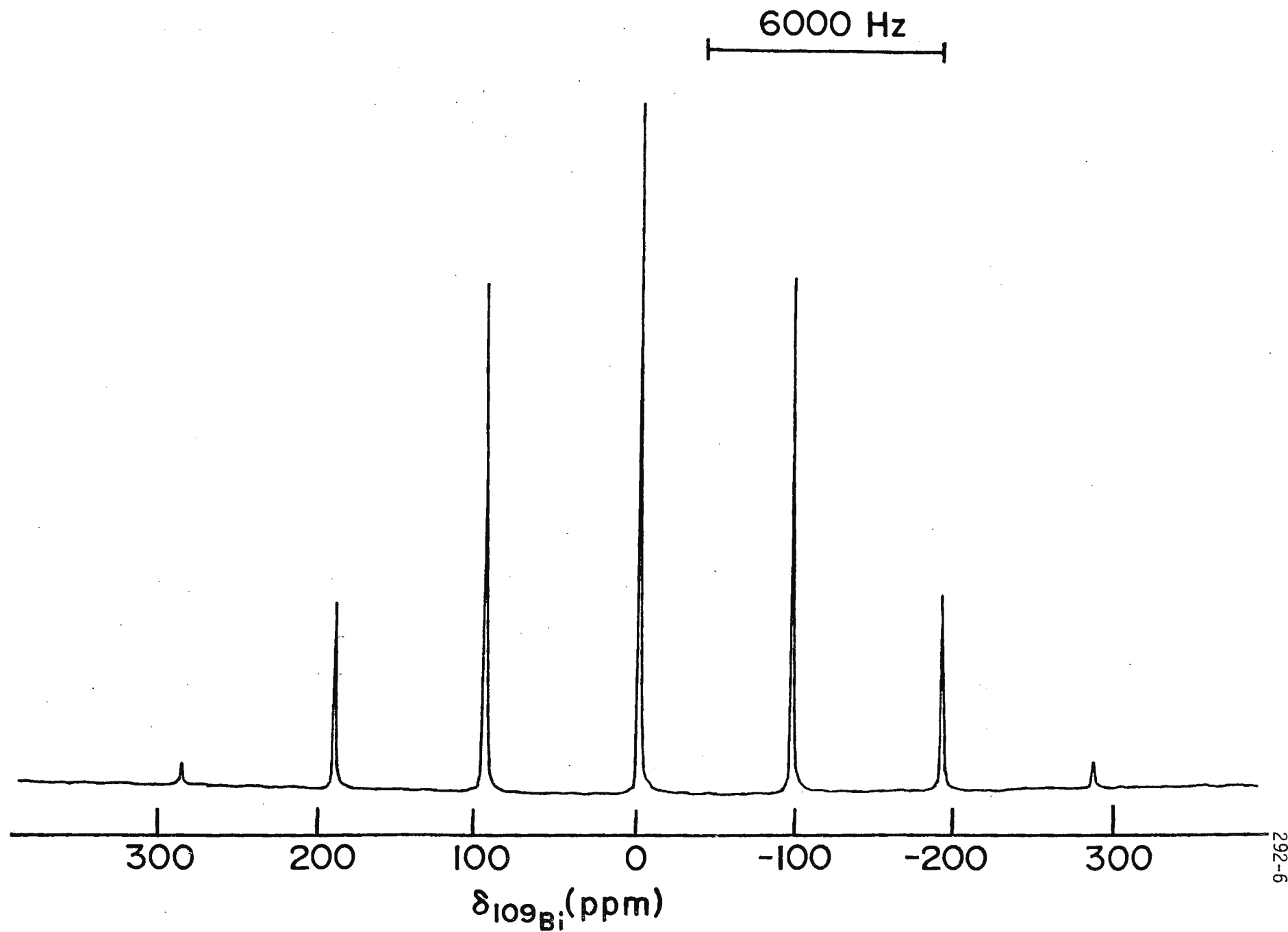
1. C. Brevard and P. Granger, "Handbook of High Resolution Multinuclear NMR" pp. 210-211, Wiley-Interscience, New York, 1981.
2. E. Fukushima, J. Chem. Phys., 55, 2463 (1971).

Please credit this contribution to the account for J.I.A. Thompson.

KM/BGS/GJS/lp



$^{209}\text{Bi}$  Spectrum of  $(\text{CH}_3)_4\text{N}^+\text{BiF}_6^-$  at 40.2 MHz.



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UNIVERSITY OF OTTAWA

December 21, 1982

Professor B.B. Shapiro  
 Department of Chemistry  
 Texas A & M University  
 College Station  
 Texas 77842, U.S.A.

Molecular wrapping of the sodium cation by a large crown ether.

Dear Professor Shapiro:

After having been a coworker of Pierre Laszlo in Liège for several years, I've left Belgium for Canada, drizzle for snow, the Flemish-French dispute for the English-French dispute and chocolate for maple syrup! Talking of maple syrup, viscosity is a parameter very often involved in NMR problems. In particular, the relaxation rate of a quadrupolar ion in solution, under some conditions, could be proportional to the reorientational correlation time describing the quadrupolar relaxation processes, and consequently, to the viscosity of the solution if the Debye-Stokes-Einstein relationship applies.

We have found such a relationship in the case of the sodium cation engaged into a crown ether wrapped around it.<sup>(1)</sup> The Na-23 relaxation rate of the sodium cation complexed by the dibenzo-24-crown-8 in mixtures of pyridine and acetone, is linearly related to the viscosity of the mixture\*. The quadrupolar coupling constant is the same for the whole range of molar fractions from which it can be calculated to be 1.0 MHz, thereby showing the expulsion of the solvent molecules from the first solvation sphere of the sodium cation. Finally, it is a very good indication of the rigidity of the coordination sphere in the time scale of the reorientational processes.

Please credit this letter to the subscription of Robert R. Fraser.

<sup>(1)</sup> M. Bisnaire, C. Detellier, D. Nadon, Can. J. Chem., in press.

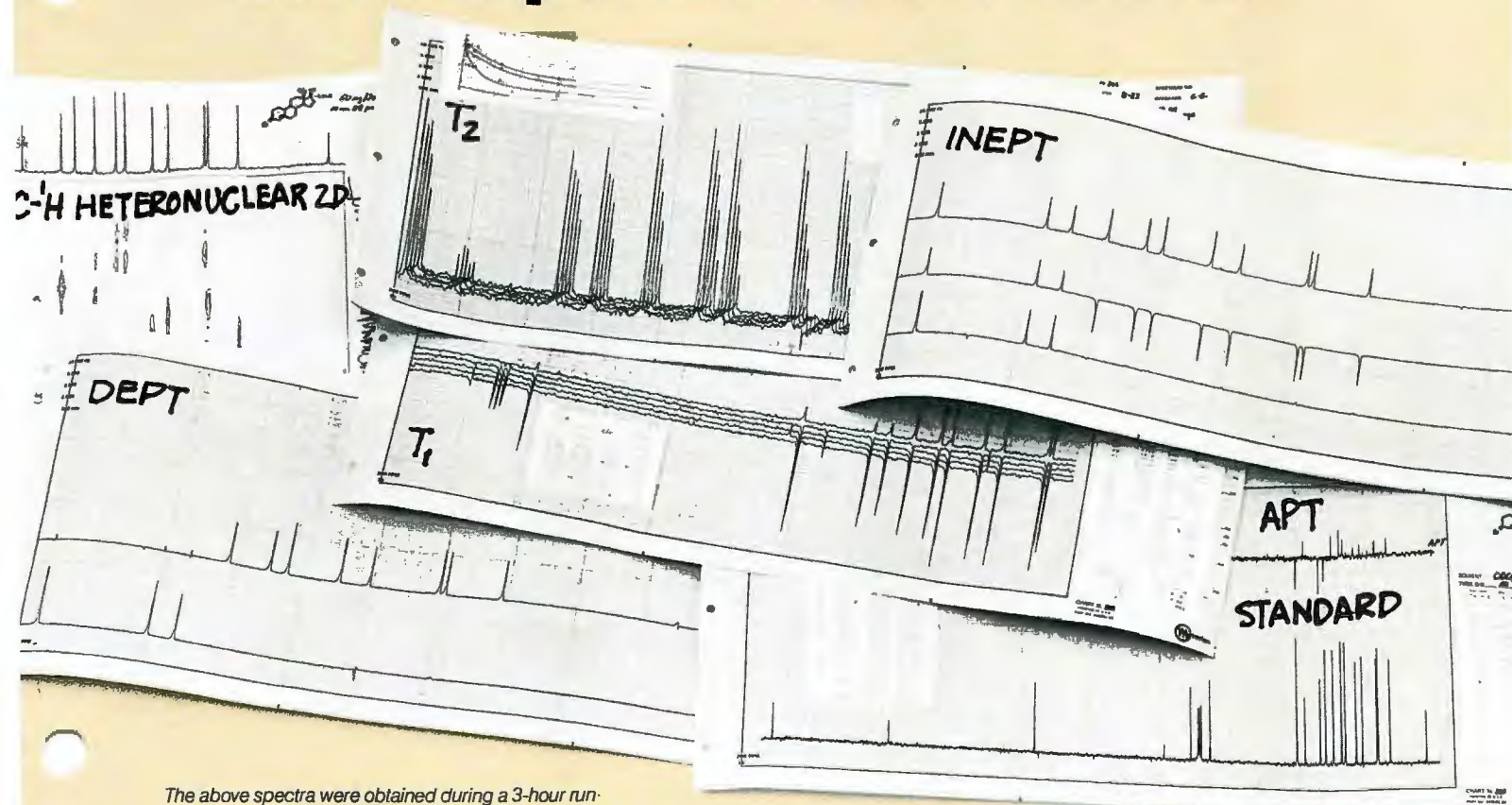
Sincerely yours,

Christian Detellier  
 Assistant Professor of Chemistry

CD:cmg

\* ( $\rho = 0.999$  for 10 points)

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Professor Bernard L. SHAPIRO  
Texas A & M University  
College of Science  
Department of Chemistry  
COLLEGE STATION, Texas 77843  
U.S.A.

Geneva, the 20th December 1982

Dear Professor Shapiro,

In response to your note of december 7th 1982, please find here after :

1. Abstract of paper recently published or accepted for publication in the near future.

WATER PROTON RELAXATION DISPERSION FOR SPIN IMAGING AND  
TOPICAL NMR IN MEDICAL DIAGNOSIS

by G.J. Béné

Published in "New techniques and applications of magnetic resonance", Proceedings of the 7th Ampere International Summer School, Portoroz, Yugoslavia, June 14-20, 1982, edited by R. Blinc and M. Vilfan, E. Kardeij University, J. Stefan Institute, Ljubljana, Yugoslavia.

We show in this paper the importance of a sufficiently precise study of the relaxation dispersion with respect to the amplitude  $H_0$  of the applied field in view of the medical diagnosis. In view of the actual state of knowledge, and of technical possibilities, the use of the NMR, as a help for medical diagnosis, implies that  $T_1$  and  $T_2$  must be measured under optimal  $H_0$  value. A condition which must be satisfied is a preliminary detailed study of the dispersion spectra of  $T_1$  and  $T_2$  of healthy and pathological tissues. These results should permit to establish with precision :

- the necessary resolution power
- the optimal choice of  $H_0$
- the necessity of measuring both  $T_1$  and  $T_2$  or only one of them

NMR medical diagnosis - Identification "in situ" du liquide amniotique sain ou pollué de femmes enceintes au cours de la grossesse par RMN en champ faible.  
Note de B. Borcard, E. Hiltbrand, P. Magnin, H. Méhier et G.J. Béné,  
transmise par P. Grivet.



Geneva, the 20th December 1982  
 Prof. B.L. Shapiro, College Station, Texas

---

Résumé :

The free precession of water protons in the earth's field after prepolarization allows the "in situ" determination of the concentration of the amniotic fluid in serum proteins and the importance of a possible pollution by meconium

To be published in Comptes-Rendus de l'Académie des Sciences(Paris)

Low field spin-spin relaxation time in intact and lysed red cells solutions: effect of membranes and hemoglobin  
 S. Conti, D.K. Lai, B. Borcard, E. Hiltbrand, P. Magnin and G.J.Béné

Abstract - Spin-spin relaxation time measurements on red cells suspensions show that, compared to the proton relaxation time, the water exchange through the cell membranes may be considered as fast even in low fields (0.5G).  
 Depending on the state of the cells, intact or lysed, such solutions give different  $T_2$  values which is explained by a compartmentation effect of the hemoglobins by the cellular membranes.  
 A different hemoglobin concentration dependence of  $1/T_2$  between human and bovine hemolysates has also been observed.

2) The announcement of the next meeting of the Ampère group

Organizer and Location :

The 6th Specialized Colloque AMPERE will be organized by the Nuclear Magnetic Resonance group of the Nuclear Research Center "Demokritos" Athens - Greece under the sponsorship of Groupement Ampere and the Greek Atomic Energy Commission. The Congress will take place in the island of Kreta, Greece, from September 12 to September 17, 1983 in "Hotel Kapsis", 25 km west from the city of Heraklion.

Scope of the Congress:

The congress is intended to be devoted partly (3days) to the study of quadrupole interactions in solids, as examined by NMR, NQR, EPR, DR and Mössbauer methods and partly (2days) to the study of magnetic resonance spin-imaging in condensed matter.  
 In both fields the emphasis will be on basic physical aspects though applications will be covered too. The scope of the Congress is to bring together leading spectroscopists and young research workers who want to become more familiar with the recent developments in these fields.

Geneva, the 20th December 1982  
Prof. B.L. Shapiro, College Station, Texas

---

Applications :

Those who intend to participate are kindly asked to return the filled pre-registration forms to the Congress Address not later than January 30, 1983. The number of participants will be limited to 200.

The registration fee will be 100US\$ or the equivalent amount in any other convertible currency. The approximate price for the Hotel from Sunday night 11.9. to Saturday morning 17.9 - double occupancy is 200US\$.

Further information with the final registration and hotel reservation will be sent with the second announcement in February 1983.

Congress address :

6th Specialized Colloque AMPERE  
Dr. F. Milia  
N.R.C. Demokritos  
Ag. Paraskevi-Attikis  
ATHENS  
GREECE

Yours sincerely,



Prof. G.J. Béné

# Mobil Research and Development Corporation

November 30, 1982

RESEARCH DEPARTMENT  
P.O. BOX 900  
DALLAS, TEXAS 75221

EUGENE L. JONES  
MANAGER  
FIELD RESEARCH LABORATORY

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

RE:  $^{29}\text{Si}$  NMR SPECTRA OF FRAMEWORK SILICATES

Dear Barry:

JEOL has recently installed a Chemagnetics SCM solids probe on our JEOL FX-270 NMR spectrometer, and we are using it to measure  $^{29}\text{Si}$  high resolution spectra in solids. The probe works quite well, and we are making very interesting measurements.

In an attempt to correlate  $^{29}\text{Si}$  chemical shifts with structural bonding parameters, we have found a linear correlation between chemical shifts ( $\delta$ , referred to TMS) and the mean silicon-oxygen ( $\langle\text{Si-O}\rangle$ ) bond distances for the Si sites in the framework silicates albite, natrolite, quartz, and cristobalite. Using our NMR data, NMR data from the literature, and bond distances from the literature, we obtained the relationship

$$\langle\text{Si-O}\rangle(\text{\AA}) = 1.6852 + 7.29 \times 10^{-4}\delta.$$

The data plotted in the attached graph show the excellent linear relationship for this set of minerals.

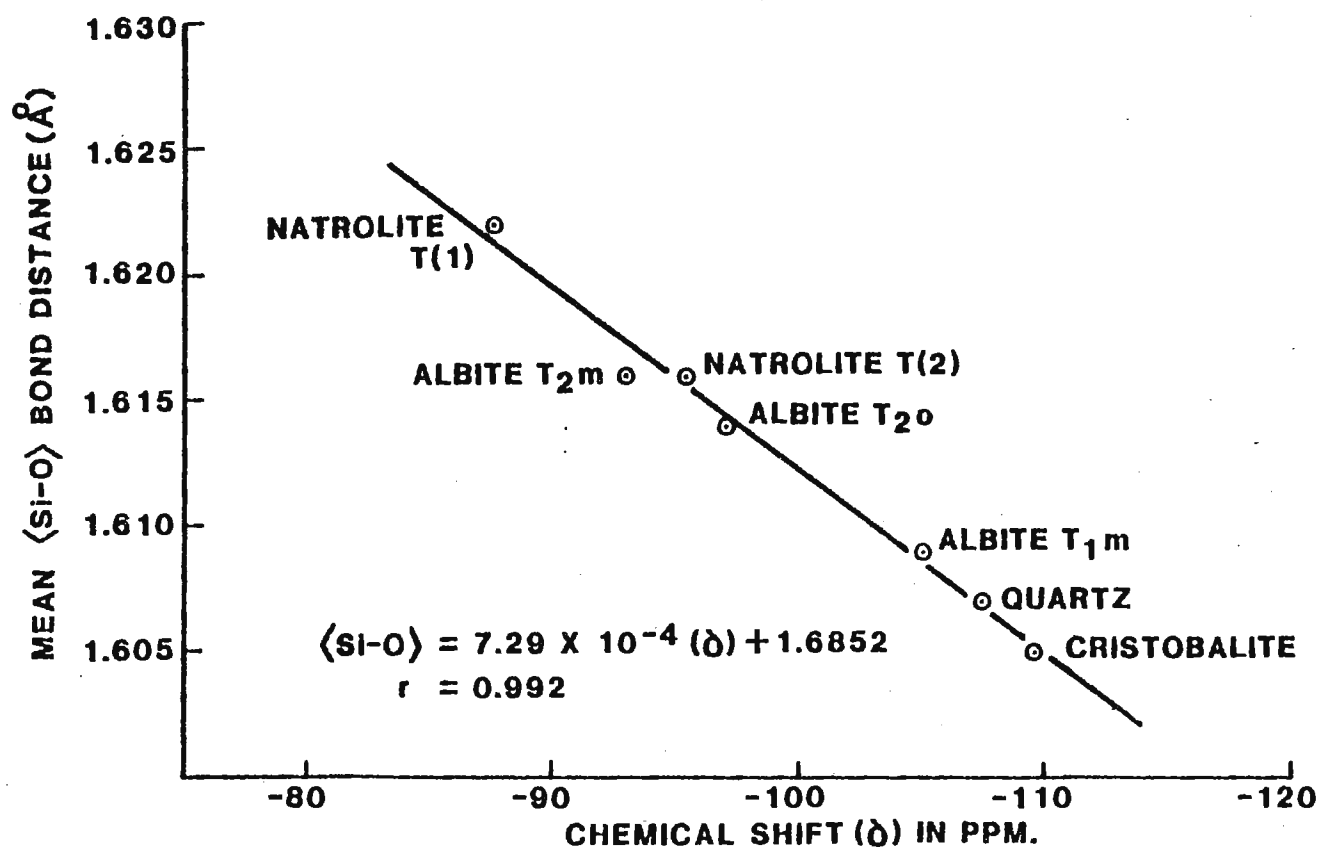
Sincerely,

*Don*

D. E. Woessner

DEW:daf  
cc E. L. Jones  
J. T. Nipper

**$^{29}\text{Si}$  NMR CHEMICAL SHIFTS ( $\delta$ ) VS MEAN  $\langle\text{Si-O}\rangle$  BOND LENGTHS  
FOR FRAMEWORK SILICATES**





December 15, 1982

TITLE: Thallium-205 nmr on a WP 100 Supercon

Dear Barry,

Our local preparative wizard, Dr. Gary Schrobilgen of McMaster University, has been making some compounds designed to warm the cockles of any spectroscopist's heart. The most recent heart warmer is a set of polyatomic anions containing thallium, tellurium and selenium. The  $^{125}\text{Te}$  and  $^{77}\text{Se}$  spectra had been observed but  $^{205}\text{Tl}$  spectra were required to provide a definitive structural assignment of the species present in solution.

The Bruker Canada Applications Lab. is equipped with two supercon spectrometers, a WM 360 and a WP 100 SY/SC, but thallium, which resonates at 206 MHz and 57 MHz respectively, is outside the 'normal' probe range of these spectrometers. The 10 mm BB probe from the 360, however, tunes over the whole range from  $^{39}\text{K}$  to  $^{31}\text{P}$  (16 to 146 MHz) and physically fits the WP 100 magnet. The WP 100 console is broadbanded; so this hybrid allows us to obtain good  $^{205}\text{Tl}$  performance ( $90^\circ$  pulse width = 10  $\mu\text{s}$ ) at 57 MHz.

The spectra in Figure 1 show the various thallium species in solution: both the natural abundance tellurium ( $^{125}\text{Te} \approx 7\% \text{ spin } \frac{1}{2}$ ) and the enriched tellurium sample ( $\approx 75\%$  enrichment) are depicted. The table below summarizes all the relevant coupling constants and chemical shifts.

Merry Christmas from the Great White North.

*Alex*

Dr. Alex D. Bain  
Applications Spectroscopist

ALB/CR/wen

*Charlie*

Dr. Charles Rodger  
Applications Chemist

Species	Chemical shift <sup>a</sup> $\delta/\text{ppm}$	Coupling constants	
		$J$ TlTe/Hz	$J$ TlSe/Hz
$\text{TlSe}_3^{3-}$	2784	-----	7250
$\text{TlSe}_2\text{Te}^{3-}$	2008	17746	7040
$\text{TlSeTe}_2^{3-}$	1204	16974	6834
$\text{Tl Te}_3^{3-}$	376	16212	----

a).  $^{205}\text{Tl}$  shift measured relative to 0.1 M thallous acetate in water.

serving to advance scientific frontiers with . . .

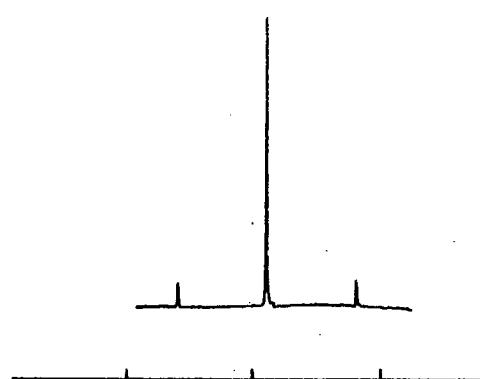
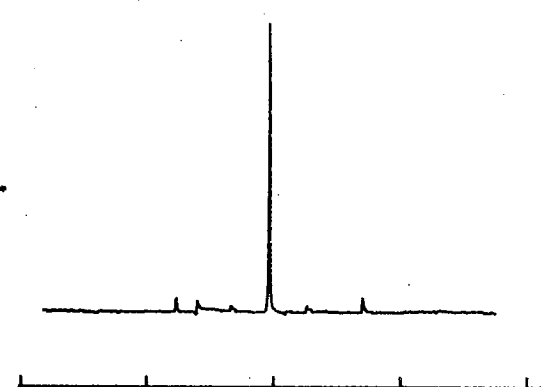
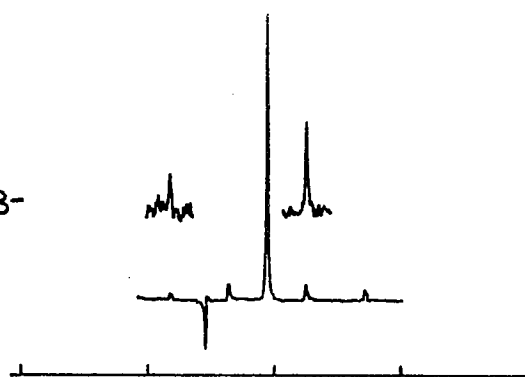
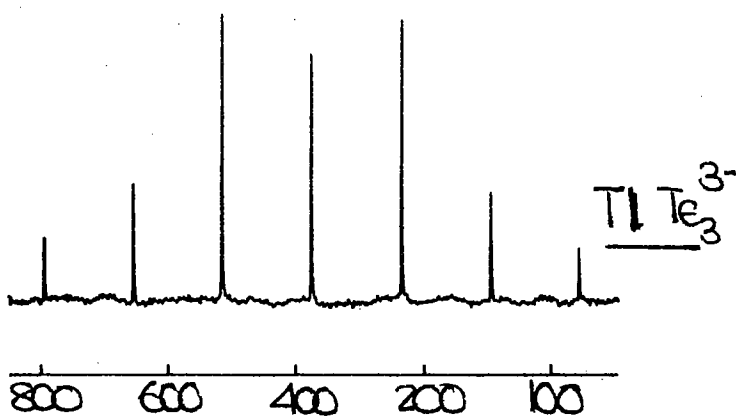
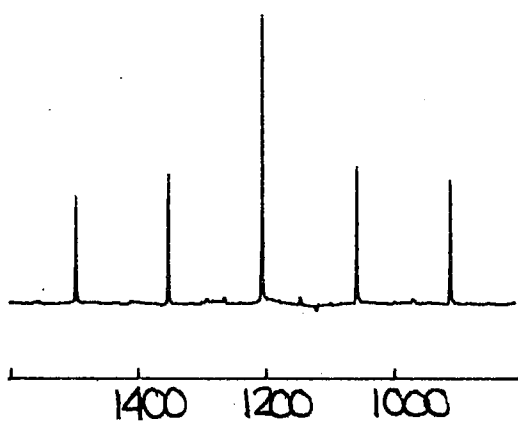
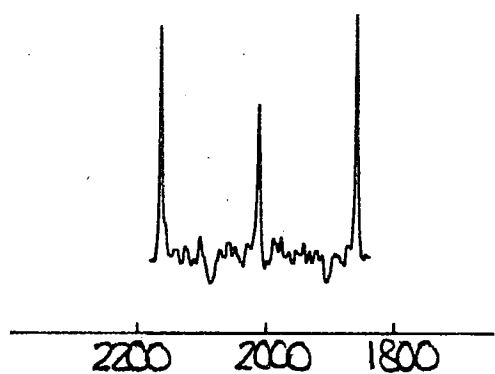
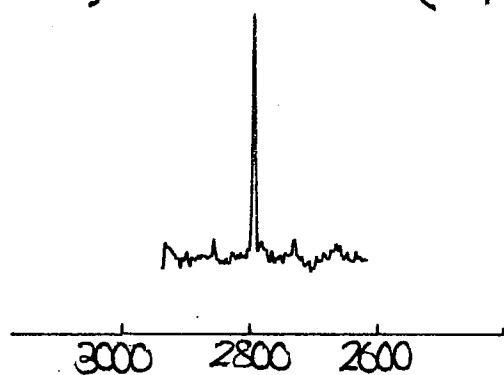
- wp/wm series high resolution electro- and cryomagnet spectrometers
- cxp series pulsed nmr spectrometers
- pc 20 series pulsed nmr process analyzers for industry
- er series epr spectrometers
- ifs series ft infrared spectrometers
- superconducting magnets/electromagnets/magnetic field measuring devices
- magnetic susceptibility systems/polarography/medical electronics
- nmr tomography medical imaging systems



Figure 1:  $57.8 \text{ MHz } ^{205}\text{Tl}$  spectra of  $\text{TlSe}_x\text{Te}_{3-x}^{3-}$

a)  $^{125}\text{Te}$  enriched ( $\approx 75\%$ )

b)  $^{125}\text{Te}$  natural abundance





# State University of Utrecht

## Laboratory for organic chemistry

Croesestraat 79  
3522 AD Utrecht  
Telefoon 030-882311  
The Netherlands

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

Date  
Your reference  
Our reference  
Subject

17 December 1982

Carbon-13 chemical shift increments for acetylenes.

Dear Professor Shapiro,

We just received your "final ultimatum letter", dated 11/11/82, hence we submit hastily this contribution, which was prepared after your first reminder, hoping we will be in time to avert the expiration of the subscription of our department.

In our laboratory the synthesis and chemical properties of unsaturated compounds, such as acetylenes, allenes and cumulenes, have been a major area of interest for many years. This has led to the availability of large numbers of acetylenes and allenes, randomly substituted with groups of different nature. This enabled us to establish for the allenes that the carbon-13 chemical shifts of the allene moiety are a constitutive property<sup>1</sup>. We now report that for the acetylenes too, the carbon-13 chemical shifts are a constitutive property. On this basis we have been able, starting from the chemical shift data of over 200 acetylenes, to establish a convenient method for estimating carbon-13 chemical shift values for the acetylene moiety.

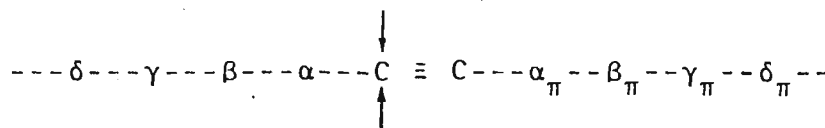
Using a multiple linear regression computer program, a set of substituent parameters was calculated for a number of the most commonly occurring groups. The calculated substituent effects for these groups (C, O, S,  $\Phi$ , N and C=C) allow a prediction of the chemical shifts of the acetylene carbons with a standard deviation of 1.54 ppm. In describing the chemical shifts, we used the following expression:

$$\delta(^{13}\text{C}) = B + \sum_{i=\alpha}^{\delta} \chi_i + \sum_{i=\alpha}^{\delta} \chi_{\pi i} + S^{\alpha} + S_{\pi}^{\alpha}$$

The base value B was estimated as 71.0 ppm in the regression analysis. The S-terms are terms which take into account the number of substituents at the  $\alpha$ -substituent. The other substituent effect terms used are depicted in the figure.

For a number of substituents the data-set was too small to apply the regression analysis. For these substituents (C=C=C, C $\equiv$ C, CHO, CO, COO, CON, Cl, Br, I, Si(CH<sub>3</sub>)<sub>3</sub>) the substituent parameters were established from a difference analysis.

In the calculation all substituent effects are taken into account. The steric correction S is applied only for the  $\alpha$ -substituents.



$$\delta = 71.0 + \sum_{i=\alpha}^{\delta} \chi_i + \sum_{i=\alpha}^{\delta} \chi_{\pi i} + S^{\alpha} + S_{\pi}^{\alpha}$$

$\delta$	$\gamma$	$\beta$	$\alpha$		$\alpha_{\pi}$	$\beta_{\pi}$	$\gamma_{\pi}$	$\delta_{\pi}$
0,4	-0,8	5,8	7,2	$-\text{C}^*$	-4,7	0,5	1,3	-0,2
	2,3	0,7	11,2	$-\text{C}=\text{C}^*$	7,5	5,5	3,3	
			4,1	$-\text{C}=\text{C}=\text{C}^*$	6,4			
-1,2	-2,7	-2,5	-1,8	$-\text{C}\equiv\text{C}-$	-6,8	3,3	2,7	0,5
	0,2	3,1	11,8	$-\text{C}_6\text{H}_5$	7,7	4,5	1,9	
			8,6	$-\text{CHO}$	14,2			
			4,3	$-\text{CO}-$	7,6			
		-2,2	2,8	$-\text{CO}-\text{O}-$	2,6	6,9		
			5,0	$-\text{CO}-\text{N}-$	6,0			
1,6	-5,0	1,9	8,1	$-\text{N}^*$	-20,0	3,6	3,4	1,3
-0,8	-3,3	2,9	14,9	$-\text{O}-$	-47,2	5,9	2,9	1,1
		1,8	-3,2	$-\text{S}-$	9,9	3,6		
1,6	-4,7	0,3	-10,8	$-\text{Cl}$	-13,4	7,3	4,9	-0,6
		0,7	-29,4	$-\text{Br}$	-3,2	8,1		
			-71,3	$-\text{I}$	10,6			
		4,6	17,0	$-\text{Si}(\text{CH}_3)_3$	23,8	3,0		

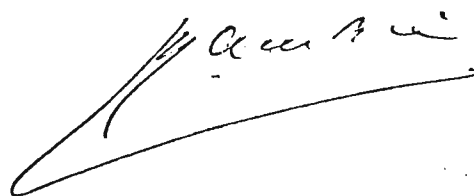
## Steric Corrections S

	$S^{\alpha}$	$S_{\pi}^{\alpha}$
$-\text{CH}_3$	0	0
$-\text{CH}_2\text{R}$ , $-\text{CH}=\text{C}^*$ , $-\text{HC}=\text{C}=\text{C}^*$ , $-\text{NHR}$	0	0
$-\text{CHR}_2$ , $-\text{CR}=\text{C}^*$ , $-\text{RC}=\text{C}=\text{C}^*$ , $-\text{NR}_2$	-2,0	-1,9
$-\text{CR}_3$	-4,0	-3,8

1. Recl. Trav. Chim. Pays-Bas 100, 85 (1981)

Yours Sincerely

M.J.A. de Bie  
H.W.A. Biessels  
J.C. Roos-Venekamp



**Laboratorium voor Technische Natuurkunde**

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

Dear Professor Shapiro:

During the last couple of years  $^{13}\text{C}$  CP(MAS) spectra have been used to characterize coal and to obtain information about its molecular structure. However, it still is a standing problem how many carbon atoms actually are observed, because both  $^{13}\text{C}$  atoms close to the free electrons and/or far away from the protons may not be measured due to respectively a large dipolar shift and a long matching time.

We used a different approach to determine this number by measuring the  $^{13}\text{C}$  relaxation behaviour in the rotating frame. This was done both for a FID-lock experiment, where a  $90^\circ$  pulse is applied before spin-locking, and a CP-lock experiment, where  $^{13}\text{C}$  spin-locking is preceded by a  $^1\text{H}$ - $^{13}\text{C}$  cross-polarization experiment, see fig.1.

Timing diagrams for two NMR experiments. (a) shows a  $^{13}\text{C}$  channel with a  $90^\circ_x$  pulse followed by a delay  $\omega_{1y}$ , and a  $^1\text{H}$  channel with a decouple pulse. (b) shows a  $^{13}\text{C}$  channel with two  $\omega_1$  delays and a  $90^\circ_x$  pulse, and a  $^1\text{H}$  channel with a match pulse followed by a decouple pulse.

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

$\omega_1 = 2.7 \cdot 10^5 \text{ s}^{-1}$ . Moreover, in both experiments Dynamic Nuclear Polarization was applied to enhance the signals (1), so that the experiments could be performed in a reasonable time (typically a few hours per experiment). Magic angle spinning was not used. From different experiments we know that the  $^{13}\text{C}$  rotating frame relaxation is determined by the free electrons. Then the theory of Tse and Hartmann (2) can be applied. They found that for spin systems like  $^{13}\text{C}$ , where spin diffusion can be neglected, the rotating frame relaxation is given by

$$S(t) = \exp \left( - \sqrt{t / T_{1\rho}^c} \right) \quad (1)$$

provided that all spins are observed. If for some reason a part  $S_1$  is not measured  $S(0)$  becomes  $S(0) = 1 - S_1$ . Moreover the exponential behaviour holds for larger values of  $t$  only.

We measured the  $^{13}\text{C}$  rotating frame relaxation of an anthracite with a

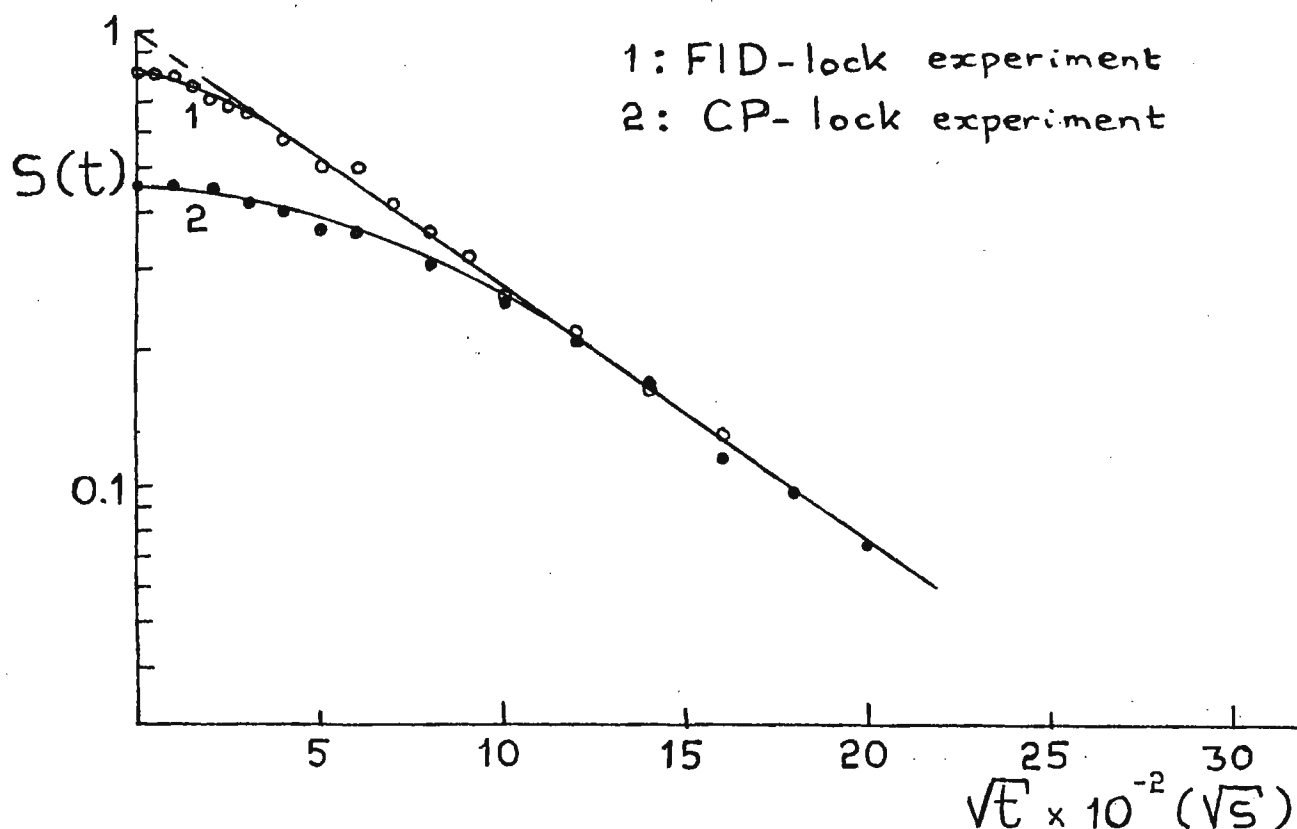


Fig.2. The  $^{13}\text{C}$  rotating frame relaxation of anthracite

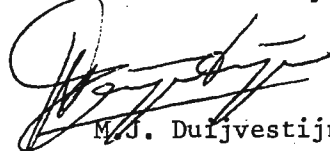


volatile matter percentage of 6% and a number of free electrons of  $4.10^{19} / \text{cm}^3$ . This coal contains almost only aromatic carbon atoms. Fig.2 shows the results. Both curves show the same final slope of  $\sqrt{T_{1\rho}^c} = 7.8 \cdot 10^{-2} \text{ } \sqrt{\text{s}}$ . It follows from the FID-lock experiment that  $S(o) \approx 0.8$ , so that 20% of the carbon atoms is not observed because of their strong interactions with the free electrons. In case of the CP-lock experiment  $S(o) \approx 0.45$ , so that an extra 25% is lost because they are too far away from the protons to be polarized (we used a matching time of 0.9 ms). Similar results were found in a high volatile and a low volatile bituminous coal. Concluding it is obvious that e.g. a quantitative interpretation of  $^{13}\text{C}$  spectra is difficult and that also values of e.g. the aromaticity can be doubtful because the signal losses of the aromatic and aliphatic carbon atoms need not be the same. A publication on this subject is in preparation. Please credit this letter to Prof. J. Smidt.



R.A. Wind

Yours sincerely,



M.J. Duijvestijn

- (1) R.A. Wind, J. Trommel and J. Smidt, FUEL 61 (1982) 398
- (2) Tse and S.R. Hartmann, Phys. Rev Lett 21 (1968) 511

## GX Report #2

# Introducing the JEOL Theory of NMR Productivity: Multi-terminals are better than one.



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DEPARTMENT OF CHEMISTRY  
TAMPA, FLORIDA 33620813:974-2144  
SUNCOM: 574-2144

82.12.10

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

Dear Barry:

Recently (for example, J. A. Peters, et al., J. Organic Chem., 46, 2784-2786 (1981)) some workers have been expressing concerns about impurities in lanthanide shift reagents. This can be serious when one realizes that a few tenths of a percent by weight of a metal such as sodium can translate into several mole percent of impurity.

It is not uncommon to have impurities such as Na(fod) sneaking into Yb(fod)<sub>3</sub>; similar problems exist with the dpm analog, Yb(dpm)<sub>3</sub>.

Since much of our work involves Eu LSR's, we decided to do a little detective work on some off-the-shelf Eu(fod)<sub>3</sub>. Sodium impurities are often thought to occur in LSR's as the sodium salt of the ligand; for example, the impurity in Eu(fod)<sub>3</sub> would be Na(fod). Much of the evidence for the existence of such an impurity lies in mass spectrometric and atomic absorption results. With these methods it is possible, however, to have sodium impurities occurring as simpler sodium salt such as NaCl. With our LSR samples, we used NMR (23-Na) to detect the sodium. The Na<sup>+</sup> signal is easily found in a dilute solution of NaOH (one pulse sufficed). It was also easily found in ca. 0.01M solutions of Na(fod). Here, less than 100 pulses gave a visible signal. Finally, after 10000 pulses on a 0.6M solution of Eu(fod)<sub>3</sub> in CDCl<sub>3</sub>, we found absolutely nothing but noise.

What was done here addresses the problem of europium LSR's only. Apparently, these are easier to keep impurities out of than is the case with ytterbium. Also, if potassium compounds were used instead of sodium, it is a little more difficult to detect the contamination by NMR. So, for quick checks of purity, it would be suggested that sodium compounds be used throughout the preparation.

Sincerely yours,

Milton D. Johnston, Jr.

G. Herbert Caines

SUGGESTED TITLE: LSR IMPURITIES--NA NMR MONITORING

Columbia University in the City of New York | New York, N. Y. 10027

DEPARTMENT OF CHEMISTRY

Havemeyer Hall

29 December 1982

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

Dear Professor Shapiro:

2-D NMR of Perfused Rat Hearts

Most readers of TAMU newsletter would agree that there have been two major developments in NMR in the last decade. One has been the investigation of intact biological tissues and organs. The other has been the introduction of the concept of two-dimensional Fourier transformation.

Here at Columbia, believing that it is impossible to get too much of a good thing! we decided to combine these two techniques, by using 2-D NMR to probe cardiac enzyme kinetics in intact hearts.

The stacked plot shows a P-31 2-D magnetization exchange spectrum from a perfused rat heart. The diagonal peaks correspond (from left to right) to inorganic phosphate, phosphocreatine and the  $\gamma$ ,  $\alpha$  and  $\beta$  resonances of ATP. The off-diagonal peaks indicate the occurrence of magnetization exchange. They occur exclusively between the phosphocreatine and the  $\gamma$  ATP peaks, thus demonstrating the action of the enzyme creatine kinase:  $\text{ATP} + \text{Creatine} \rightleftharpoons \text{ADP} + \text{Phosphocreatine} + \text{H}^+$ .

Unfortunately, the data acquisition takes about 11 hours, so our major concern at present is to find a way to improve the sensitivity.

Yours Sincerely,

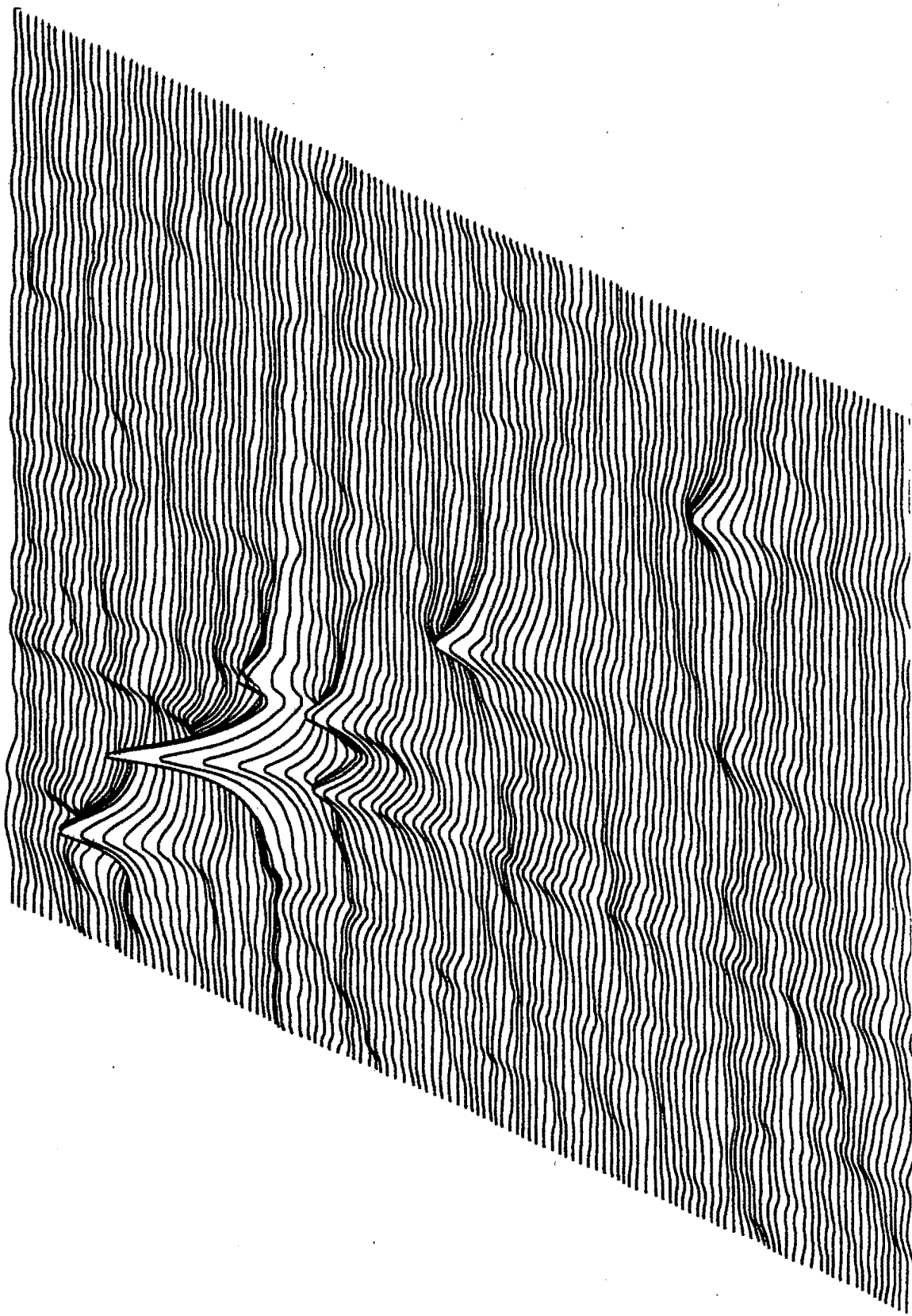


C. J. Turner  
Department of  
Chemistry



P. B. Garlick  
Department of  
Pharmacology





SADIS BRUKER SPECTROSPIN, Boîte Postale N 67160 WISSEMBOURG

## Départements :

Spectrométries de Résonance Magnétique

Spectrométrie Infra-Rouge Fourier

Polarographie

Aimants &amp; alimentations stabilisées

Mesures de Susceptibilité magnétique

Recherche Océanographique

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

N./Réf.  
 V./Réf.

82 12 449 CB/AMB

Wissembourg, le

December 29th 1982

TUNGSTEN NMR : DIRECT OBSERVATION OF THE  $W(CO)_6$  RESONANCE

Dear Barry,

Tungsten NMR has proven to be a valuable structural and analytical tool for chemists (1). Although complete sets of data exist for  $W(CO)_{6-x}(PR_3)_x$  and related compounds (2), the  $W(CO)_6$  chemical shift was still unavailable in the literature, except a guessed value from a correlation of chemical shifts in phosphine substituted tungsten carbonyl complexes (2a).

We were able to obtain directly the  $W(CO)_6$  chemical shift value in both solid and solution state on a WM 400 (16,67 MHz for 183 W).

The solid state spectrum was obtained with a 10 mm tube filled with  $W(CO)_6$  (66 pulses 16 hours !!). The liquid state one is a by-product of a research programme we undertook in collaboration with Prof. J. Riess' group in Nice on Phosphorus cage compounds. Interestingly enough, the chemical shift anisotropy of the Tungsten site in the solid is not very high (" $\Delta\nu_{1/2}$ " = 500 Hz) and its chemical shift (-3440 ppm) is very close to the chemical shift of  $W(CO)_6$  in solution : - 3447 ppm (from  $WO_4^{2-}$  1M in  $D_{2O}$ ), suggesting very small environmental interactions on the  $W(CO)_6$  moiety from solid to liquid state.

.../...



.../...

The chemical shift we found for  $W(CO)_6$  in solution is in good agreement with the shift expected by Mc Farlane et al (2a) :

-  $2400 \pm 40$  ppm from  $WF_6$  or -  $3521 \pm 40$  ppm from  $WO_4^{2-}$  1M in  $D_2O$ .

I hope you have relaxed from these two hectic weeks in Stirling and I wish you a very good 1983 year.

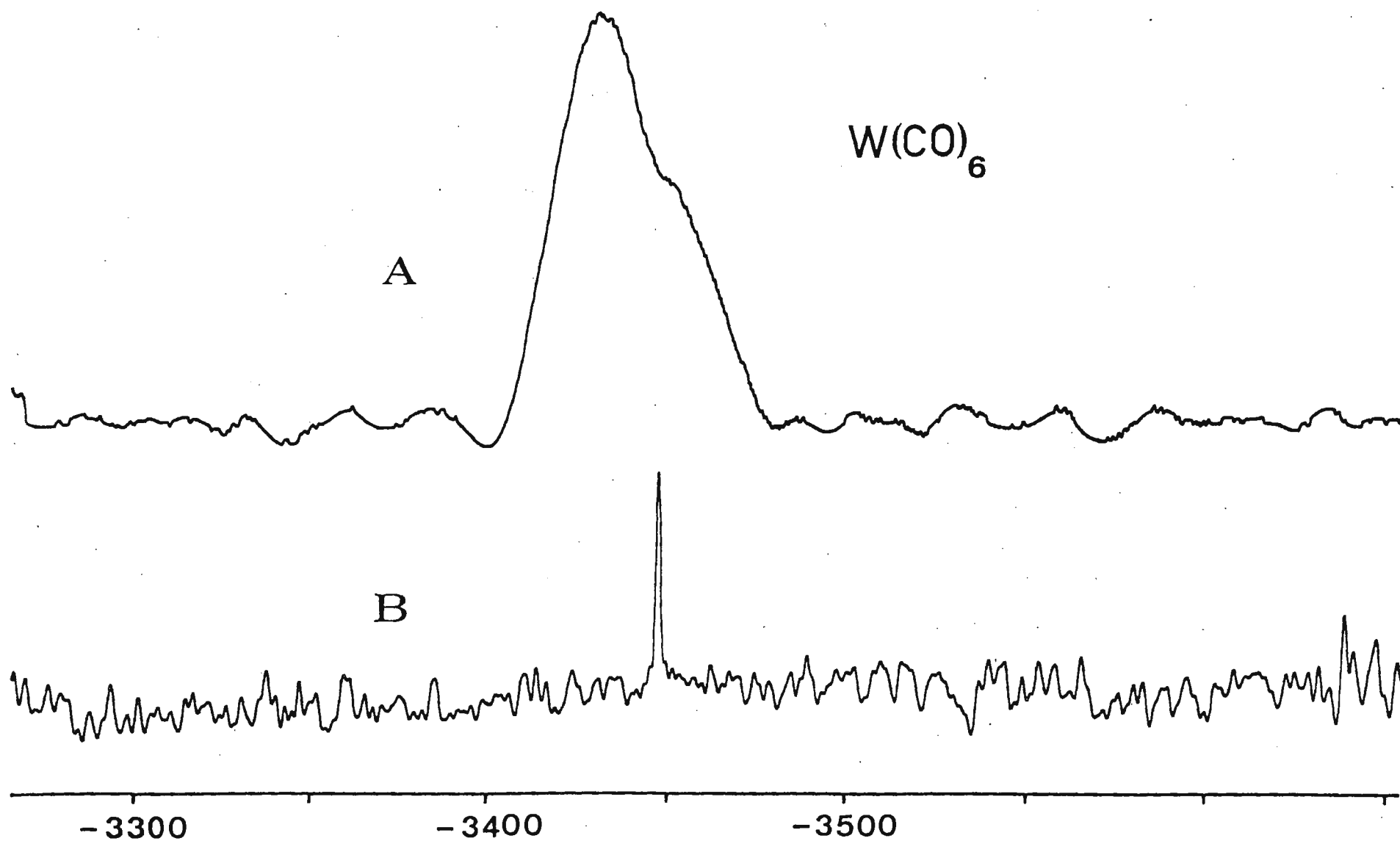
C. BREVARD

Christian

- 1) a : NMR and the Periodic Table. R.K. Harris, B.E. Mann.  
Academic press (1978).  
b : C. Brevard, J. Lefebvre, F. Chauveau, P. Doppelt.  
J. Am. Chem. Soc. 103, 4589 (1981)
- 2) a : H.C.E. Mc Farlane, W Mc Farlane, D.S Rycroft, J. Chem soc  
Dalton Trans. 1616 (1976)  
b : NMR and the Periodic Table. R.K. Harris, B.E. Mann.  
Academic press (1978). Pages 215-217.

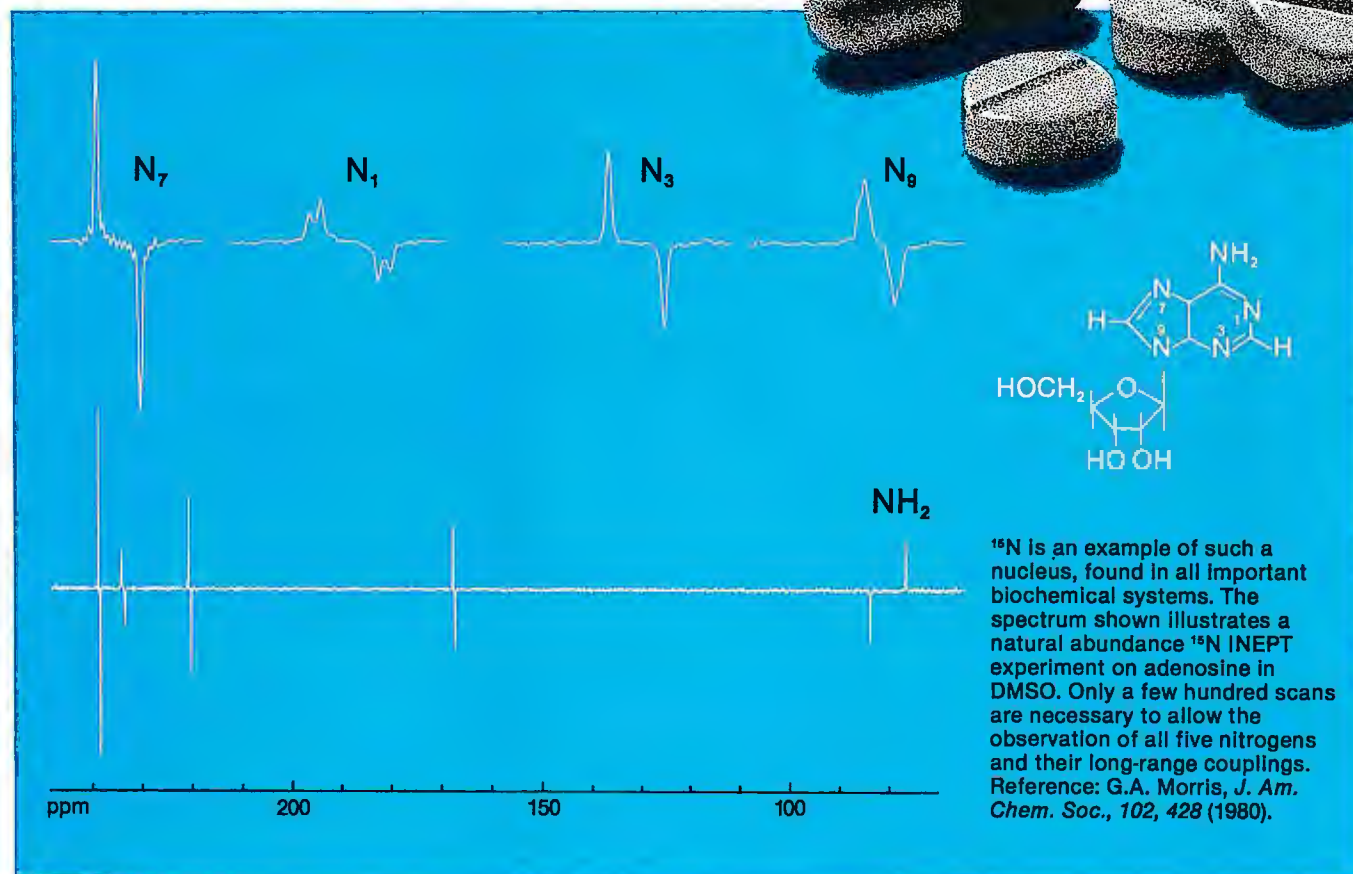
183 W Spectrum of  $\text{W(CO)}_6$ , 16,6 MHz (ref. :  $\text{WO}_4^{2-}$  1 M in  $\text{D}_{20}$ ).

A : solid state spectrum : 66 pulses, 900 s waiting time, 30  $\mu\text{s}$  pulse ( $90^\circ$ ), 10 mm tube.  
B : solution state spectrum : fast pulsing mode,  $2 \cdot 10^6$  scans,  $90^\circ$  pulse, 0,03 sec. AQT,  $\sim 10^{-2}$  M in Toluene  $\text{d}_8$ .



# Efficient $^{15}\text{N}$ studies by NMR

Low gamma nuclei are often difficult to detect directly because of their low sensitivity, long  $T_1$ 's, and unfavorable NOE's. However, using the INEPT technique, signal intensity can be borrowed from the abundant coupled proton spins through a process called "magnetization transfer," allowing their direct observation.



**Q.E.D.** The above INEPT experiment was performed on a routine NMR spectrometer at the Bruker Applications Laboratory. The new AM Series of high-field NMR spectrometer systems comes with an extensive software system, including programs for INEPT processing, display and plotting. A new 8-color graphic display processor further facilitates speed of analysis and clarity of data presentation.

Please tell us your particular application and ask for more information with the coupon below: Bruker Instruments, Inc., Manning Park, Billerica, MA 01821.

NMR Systems designed to solve problems.



My NMR application is: \_\_\_\_\_

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Tell me more about

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☐ NMR in Solids (CXP Series)  
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# New Literature Available from BRUKER

## NMR-Tomography

— A simple introduction into a fascinating NMR technique —

The "NMR-Imaging" technique is without any doubt a revolutionary new method for obtaining pictorial information about internal structures e.g. of the human body. The evolution of this method has now reached the state where non-specialists have recognized the extraordinary power of this technique and consequently BRUKER has now available an introductory six-page brochure for those not familiar with this new method. In order to facilitate the understanding of the physical background to this method the basic principles are given in a simplified manner and are illustrated by a large number of figures.

In a short survey it is shown that for the last twenty years the instrumental development in the pulsed NMR field has been synonymous with the name of BRUKER and it is pointed out that the first commercially available Fourier Transformation (FT) spectrometers were developed by BRUKER in 1969. Since NMR tomography is based on both "pulsed" and "FT"-NMR, the unique experience of BRUKER in these fields represents the ideal basis for the recently developed imaging systems.

After a short introduction, the principles of NMR are described in the brochure followed by a short representation of the "Projection-Reconstruction-Technique". Due to the expected extraordinary importance of NMR tomography in the field of diagnostic medicine a comparison of the average X-ray tissue contrast with NMR data is given as well as some remarks about theoretically possible risks for patients. At the end of this brochure an "outlook" is given into new applications and of the expected development of NMR tomography.



The three new BRUKER brochures.

With the general title "BRUKER Info", periodically illustrations of BRUKER's latest results are added to the NMR Tomography brochure.

If you wish to obtain the new brochure containing two "BRUKER Info" illustrations please return the reply card.

## Two-Dimensional NMR aspect 2000

A practical introduction into this new technique by an experienced spectroscopist.

The common 2-D experiments are described, measuring conditions and microprograms are given. Application examples on various spectrometers demonstrate the capabilities of the method and naturally the outstanding performance of BRUKER spectrometers in 2-D spectroscopy.

## DEPT

Distortionless Enhancement by Polarization Transfer

A new method with significant advantages over other polarization transfer techniques is described in a new brochure.

This method developed at the Griffith University by Drs. Bendall, Doddrell and Pegg can be performed on any BRUKER Spectrometer equipped with a CXP or high speed pulse programmer. Using this sequence the sensitivity in coupled spectra can be significantly increased or the multiplicity selection in  $^{13}\text{C}$  spectra can be performed without the critical adjustments required for other polarization transfer pulse sequences.

For Your Copy, Please Write to Your Nearest BRUKER Sales Office



## Your reference

Your letter of

Our reference 82/100 aj/mk

Date December 6th, 1982

Enclosures

Dr Bernard L. Shapiro

Department of Chemistry

Texas A &amp; M University

College Station, TX 77843

U.S.A.

**Subject** Improvement of the signal-to-noise ratio of the CXP300  $^2\text{H}$  lock receiver.

Dear Dr. Shapiro,

The noise of the CXP300  $^2\text{H}$  lock receiver originate mainly in the wide-band amplifier. The noise at 46.1 MHz (the signal frequency) and at 18.4 MHz (the first image frequency) is heterodyned in the first mixer with 32.2 MHz (the first local oscillator frequency) to produce noise at 13.8 MHz (the first intermediate frequency 1 IF). We have added a selective filter between the broadband amplifier and the first mixer to suppress the image noise. A simple notch filter at 18.4 MHz gives in our CXP300 an improvement of the signal-to-noise ratio of the lock signal of about 70%.

We connect the cable from the probe directly to the receiver and not to the rear panel, reducing the leakage of stray radiation into the cable.

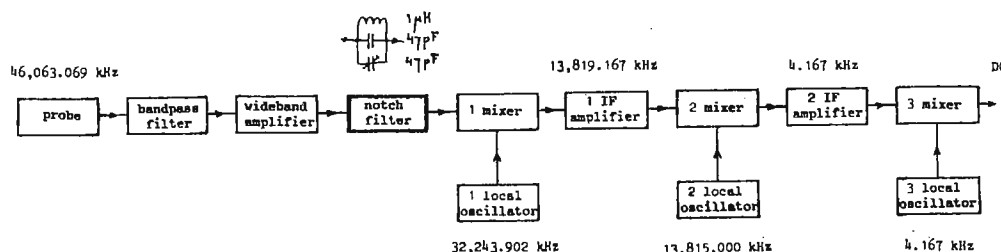
A further improvement of the signal-to-noise ratio can be obtained by suppressing the second image noise and other spurious responses. Because the image frequency is very close to the signal frequency (-8.333 kHz) a very selective (crystal) filter should be required.

Perhaps similar filters can be fitted in other (Bruker) receivers to improve their noise performance.

Please credit this contribution to prof.dr. T.J. Schaafsma.

Sincerely,

P.A. de Jager.



## UNIVERSITY OF CALIFORNIA, SAN FRANCISCO

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SANTA BARBARA • SANTA CRUZ

SCHOOL OF PHARMACY  
DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

SAN FRANCISCO, CALIFORNIA 94143

December 1, 1982

Dr. Bernard L. Shapiro  
Department of Chemistry  
Texas A & M University  
College Station, Texas 77843Re: Post-doctoral and Technical Positions Available in  
Biomedical NMR

Dear Dr. Shapiro:

A significant research effort has been initiated at UCSF utilizing NMR in the areas of in vivo biochemistry and pathology (including human). The research has biomedical promise, but will require input from individuals of varying background ranging from physics and engineering through chemistry to biology and medicine for full development of that promise. Consequently, we anticipate hiring individuals immediately and during the course of the next year. We need people who can adapt and develop new NMR techniques (perhaps 2D NMR and solid state NMR) to obtain biochemical information on living animals and humans as well as more biochemical- and medically-oriented people to make some sense from in vivo NMR experiments. An effort will be made to merge the NMR spectroscopic and imaging modalities for biochemical purposes.

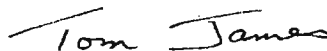
Several individuals at UCSF will be collaborating with us on this enterprise, with a strong interest in the cellular metabolism, organ function, and possible clinical use of NMR in studies of heart, kidney, and brain. For certain aspects of the work, a close collaboration with the NMR imaging lab here at UCSF (Radiology Department; Drs. L. Crooks and L. Kaufman) will be maintained.

We are in the process of acquiring three new NMR spectrometer systems for these purposes. (1) Topical NMR system, 1.9 Tesla, 200 mm usable bore for animal and human limbs, operational in February, 1983; (2) 6.3 Tesla, 84 mm usable bore system for live, healthy animal experiments with a surgically-implanted rf coil around an organ (present experiments give S/N equal to topical NMR), operational in April, 1983; and (3) topical NMR system, 1.9 Tesla, 600 mm usable bore for human NMR experiments, hopefully operational in about a year.

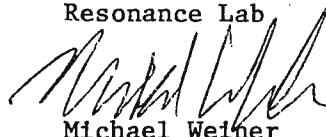


Will you please have any prospective applicants send a c.v. and arrange for three letters of recommendation to be sent to T.L. James. I request that you please post or circulate this letter.

Sincerely,



Thomas L. James  
Associate Professor of Chemistry  
and Pharmaceutical Chemistry  
Director, UCSF Magnetic  
Resonance Lab



Michael Weiner  
Associate Professor of Medicine  
UCSF

---

**BOSTON COLLEGE**  
CHESTNUT HILL, MASSACHUSETTS 02167

(617) 969-0100

DEPARTMENT OF CHEMISTRY

December 9, 1982

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

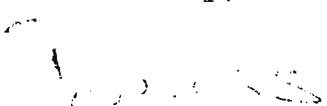
Dual Frequency FT-80A Probe For Sale

Dear Barry:

We would like to sell a dual frequency  $^{13}\text{C}/^1\text{H}$  probe for a Varian FT-80A spectrometer. Insets include a 5 mm dual frequency insert and both  $^{13}\text{C}$  and  $^1\text{H}$  1.7 mm micro inserts, neither of which has ever been used. The 10 mm insert is damaged, but may conceivably be repairable. The probe and inserts are three years old, but have been in storage since we added our broadband probe two years ago.

Interested parties should write to me.

Sincerely,



Dennis J. Sardella  
Professor of Chemistry

Dr. P. Rösch  
MAX-PLANCK-INSTITUT  
FÜR MEDIZINISCHE FORSCHUNG  
ABTEILUNG BIOPHYSIK

6900 HEIDELBERG 1, 22.12.1982  
JAHNSTRASSE 29 265  
TELEFON (06221) 496.....  
TELEX 461505

Prof. B. Shapiro  
Department of Chemistry  
College Station  
T e x a s 77843  
USA

Dear Prof. Shapiro,

your final ultimatum letter stirred my conscience to the extent that I put pen to paper and try to explain the delay:

We are currently upgrading our instrumentation. So far we shared a Bruker HX 360 spectrometer with the Department of Organic Chemistry and the Department of Molecular Physics on a host and guest basis. ( We were the guests! ) With the coming up of new projects we felt strongly the necessity of obtaining an instrument for biophysical purposes only. We were lucky enough to get the money for new instrumentation inspite of our running down economy. The final decision fell on a custom made multi purpose Bruker CXP 360 spectrometer, which will be delivered in January 1983.

Its special features:

Full multinuclear capability from 16 MHz ( $^{109}\text{Ag}$ ) to 146 MHz ( $^{31}\text{P}$ ) in both high resolution and high power mode  
 $^{31}\text{P}$  -  $^{31}\text{P}$  decoupling facility

The biochemists in our department are somewhat scared by the 20 mm probes, but I hope that we are able to report first results soon.

Best wishes for 1983 to all readers of the TAMU-NMR Newsletter!



Paul Rösch



United States  
Department of  
Agriculture

Agricultural  
Research  
Service

Northeastern Region  
Eastern Regional  
Research Center

600 East Mermaid Lane  
Philadelphia  
Pennsylvania  
19118

December 6, 1982

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

Dear Dr. Shapiro:

We have an opening in the Spectroscopy Group of the Physical Chemistry and Instrumentation Laboratory at the Eastern Regional Research Center for a Research Associate with a background in  $^{13}\text{C}$  solid state NMR spectroscopy of biomolecules and physical biochemistry. The project will involve the study of protein components and intact connective tissue with CP-MAS  $^{13}\text{C}$  NMR. Emphasis will be focused on the effects of enzymatic and/or chemical treatment to the structural integrity and molecular dynamics of these interacting systems. Knowledge of 2D NMR methods, for evaluating intermolecular spin diffusion and homogeneous broadening, would be desirable. Our facility presently has a JEOL FX60QS spectrometer capable of doing both  $^{13}\text{C}$  and  $^{31}\text{P}$  in the solid state as well as  $^1\text{H}$ ,  $^2\text{H}$  and  $^{31}\text{P}$  solution work. In mid-February we will acquire a JEOL GX-400 which will be interfaced to our lower field solids instrument. The extensive 2D capabilities of the GX-400 will then be available for the analysis of our solid state studies.

We hope to fill this position by late June or July. The salary will be \$24,508.00 per 12 months. Interested applicants should send their inquiries and resumes to me.

Sincerely,

PHILIP E. PFEFFER  
Spectroscopy Research  
Physical Chemistry and Instrumentation  
Laboratory



The Ohio State University

Department of Chemistry

140 West 18th Avenue  
Columbus, Ohio 43210

Phone 614 422-2251

December 7, 1982

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

Dear Barry,

My colleague, Professor Berliner sends the enclosed announcement.

Yours sincerely,

Gideon Fraenkel  
Professor of Chemistry

Is

Postdoctoral Position

(Biophysical Chemistry), Ohio State University

Dr. L. J. Berliner has several postdoctoral positions available for Ph.D. graduates interested in some challenging biophysical problems. We are very well equipped here. His lab has an SLM fluorescence lifetime polarization instrument, Varian E-4 ESR spectrometer and data system. NMR equipment includes Bruker WP 200 and WM 300 spectrometers.

The proposed work involves magnetic resonance (NMR, ESR), fluorescence and chemical modification studies of two different enzyme systems as an approach to mapping their topography and characterizing their function(s) in more detail. Some enzyme isolation is also required.

1. Lactose synthetase: the enzyme galactosyl transferase has profoundly altered specificity when complexed in the mammary gland cellular environment with the "lysozyme like" protein,  $\alpha$ -lactalbumin. Our studies are attempting to define the structural changes induced in each subunit of this novel catalytic-regulatory two protein complex.
2. Human  $\alpha$ -thrombin: this key blood clotting enzyme in the coagulation cascade has several unique functions, many of which are yet to be defined in structural detail. While thrombin is very much a "trypsin-like" serine protease, its restricted specificity and yet unsolved crystal structure presents a unique challenge to structural studies in solution.

Starting date: Open. Salary: \$13,320/year (minimum) or up depending upon qualifications.

Interested applicants should forward a c.v. including copies of publications and two or three references to:

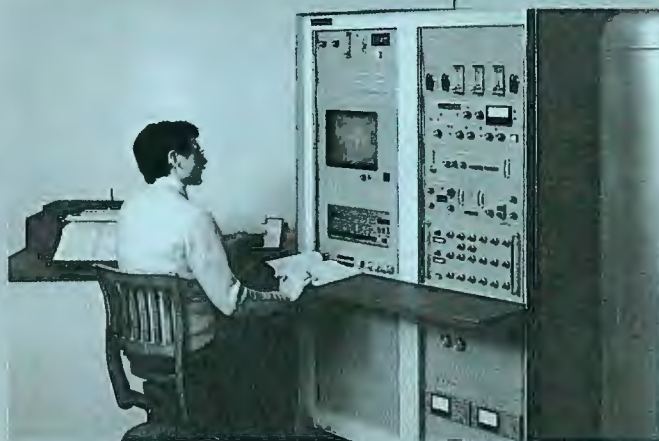
Dr. Lawrence J. Berliner  
Department of Chemistry  
The Ohio State University  
140 West 18th Avenue  
Columbus, Ohio 43210 U.S.A.

Telephone: 614-422-0134

# Examine its capabilities. Think of yours.

## **Advanced Nicolet Data System**

The new 1280 Data System and its predecessors are the most popular spectroscopy computer systems ever designed. The 1280 comes complete with 128K/20-bit RAM memory ex-



pandable to 256K. It also includes the Model 293C Pulse Programmer and the most comprehensive FT-NMR software available today.

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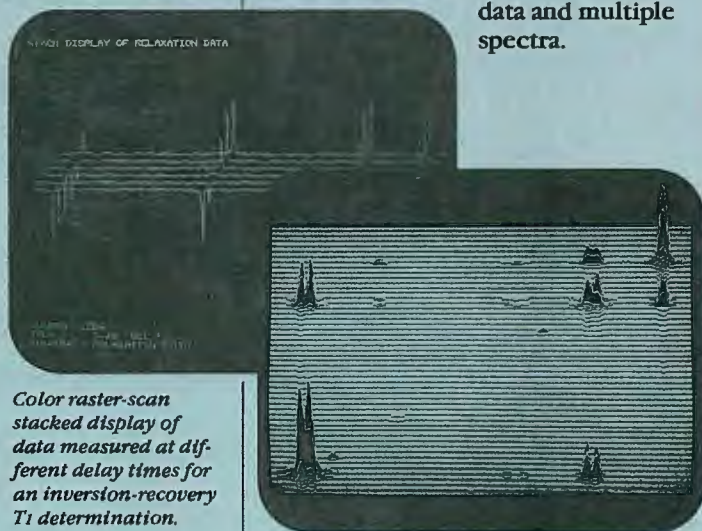
Magnets range from 4.7T to 11.7T (200, 300, 360 and 500 MHz) in both wide and narrow bore. Probes available include fixed-tune, broadband, special cross-polarization/magic angle spinning and the new sideways-spinning solenoidal.

## **Compu-Shim**

Performs fast, efficient, automatic shimming of all spin and non-spin gradients, using the lock level or FID response. Available as an option.

## **<sup>13</sup>C Library & Search Programs**

A library of 8,960 <sup>13</sup>C spectra is available, known as the EPA/NIH/NIC CNMR Data Base. Three different routines are provided to search for spectra.



*Color raster-scan stacked display of data measured at different delay times for an inversion-recovery T<sub>1</sub> determination.*



*New solenoidal sideways-spinning probes provide enhanced sensitivity.*

## **New Color Raster-Scan Display**

Optional feature provides simultaneous display of up to seven colors and full alphanumerics. Particularly valuable for displaying 2D-FT data and multiple spectra.

*Raster-scan display of 2D-FT data.*

## **"LOG IN PLEASE"**

Now update your software by phone! If you have a NIC-1180 or 1180E/1280 Data System with a 300 baud modem, we can update your software with our Telephone Software Distribution Network.

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$^{29}\text{Si}$  (~40 MHz)

with one probe!

- Self starting rotor/stator design!
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