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NOTICES

- i) See new address for the Newsletter, on p. 1.
- ii) See notice re 1987-88 subscription invoices, on p. 32.

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**FORTHCOMING NMR MEETINGS**

**Symposium on the High Resolution NMR of Solids** - October 15, 1987; Washington University, St. Louis, Missouri. See page 42 of Newsletter #346, July 1987 for additional information.

**Symposium on Resonance in Perspective - A Tribute to Professor Richard E. Norberg** - October 16-17, 1987; Washington University, St. Louis, Missouri. See page 43 of Newsletter #346, July 1987 for additional information.

**Magnetic Resonance Spectroscopy for Clinicians** - October 18, 1987; San Francisco, California; University of California Medical Center, San Francisco, California; For registration information, call (415) 476-5808.

**1987 Materials Research Society, Fall Meeting** - Nov. 29-Dec. 5, 1987; Boston Marriott Hotel, Boston, Massachusetts. Short course on NMR Spectroscopy - Wednesday, December 2. Course Instructor: James P. Yesinowski (Cal Tech). For further details, contact: Materials Research Society, 9800 McKnight Road, Suite 327, Pittsburgh, Pennsylvania 15237.

**Fritz Haber International Workshop on Modern Techniques in Magnetic Resonance** - December 13-17, 1987; Weizman Institute of Science, Rehovot, Israel; See page 7 of Newsletter #341, February 1987, for additional information.

**NMR-88** - February 14-18, 1988; Thredbo Alpine Hotel, Thredbo, N.S.W. Australia. Chairman: Dr. L.R. Brown, The Australian National University. For further information, contact: Leslie Harland, Research School of Chemistry, The Australian National University, Canberra, A.C.T. 2601, Australia. Telex: AA62172. Facsimile: (61-62)-49-7817. Telephone: (61-62)-49-2863.

**29th ENC (Experimental NMR Conference)** - April 17-21, 1988; Rochester, New York; Chairman: Professor Stanley J. Opella, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104, (215) 898-6459. For information, contact Professor Edward O. Stejskal, ENC Secretary, Department of Chemistry - Box 8204, North Carolina State University, Raleigh, North Carolina 27695-8204; telephone (919) 737-2998.

**9th EENC (European Experimental NMR Conference)** - May 16-20, 1988; Bad Aussee, Austria; For further information, write Professor H. Sterk, Karl-Franzens-Universität Graz, Institut für Organische Chemie, Heinrichstrasse 28, A-8010 Graz, Austria. See page 15 of this issue of the Newsletter.

Additional listings of meetings, etc., are invited.

All Newsletter Correspondence  
 Should be Addressed to:

Dr. Bernard L. Shapiro  
 TAMU NMR Newsletter  
 966 Elsinore Court  
 Palo Alto, CA 94303 U.S.A.

**DEADLINE DATES**

No. 350 (November) ---- 23 October 1987  
 No. 351 (December) --- 20 November 1987  
 No. 352 (January) ---- 18 December 1987



$^{17}\text{O}$  and  $^{14}\text{N}$  NMR Experiments on Nitric Acid Systems at 4.7T

August 3, 1987

(Received 11 August 1987)

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

Dear Barry:

$^{17}\text{O}$  NMR spectra have been obtained from nitric acid samples that contained added  $\text{H}_2\text{O}$ ,  $\text{N}_2\text{O}_5$ ,  $\text{KNO}_3$ , or  $\text{N}_2\text{O}_4$ . When the additive is  $\text{H}_2\text{O}$  or  $\text{N}_2\text{O}_4$  more than one NMR peak is observed. When  $\text{N}_2\text{O}_5$  or  $\text{KNO}_3$  is added a single resonance is observed.

We have examined 3.1M, 10M, and 21.8M aqueous  $\text{HNO}_3$  solutions and in each case find two  $^{17}\text{O}$  peaks. One is due to " $\text{H}_2\text{O}$ " and the other to " $\text{HNO}_3$ " oxygen environments. The chemical shifts of the  $^{17}\text{O}$  resonances, referenced to the  $^{17}\text{O}$  position for bulk water, are given in Table 1. The chemical shift for "water" molecules varies with its concentration in nitric acid. At a concentration near 10 molar nitric acid, the water most nearly resembles  $\text{H}_3\text{O}^+$ . At low and high water concentrations most of the water appears to be unionized.

If  $\text{N}_2\text{O}_5$  is added to anhydrous nitric acid in the amount of 20 wt %, still only a single  $^{17}\text{O}$  NMR peak is observed. Its chemical shift is slightly upfield from that of the anhydrous acid, 394.6 ppm vs 407.9 ppm, respectively.

Dinitrogen pentoxide is known to be highly ionized according to equilibrium (1) in nitric acid solution. This equilibrium together with equilibria (2) and (3) provide a mechanism



for rapid chemical exchange of oxygen atoms. An exchange, rapid on the NMR timescale, would explain why we observe only a single  $^{17}\text{O}$  NMR signal.

Dinitrogen pentoxide is known to decompose in anhydrous nitric acid to form  $\text{O}_2$  and  $\text{N}_2\text{O}_4$  (4).



The oxygen formed is paramagnetic and causes a change in the bulk magnetic susceptibility of the sample. This is easily monitored by  $^1\text{H}$  NMR chemical shift vs time measurements. The  $^{17}\text{O}$  NMR peak was insensitive to this decomposition. The signal from a 20%  $\text{N}_2\text{O}_5$ /80%  $\text{HNO}_3$  sample did not shift during a 5 hour decomposition period at ambient temperature.

In dinitrogen tetroxide/ $\text{HNO}_3$  solutions, integration of the  $^{17}\text{O}$  resonances for molecular  $\text{N}_2\text{O}_4$  (486 ppm) and for the combined  $\text{HNO}_3$ ,  $\text{NO}_3^-$  and  $\text{NO}^+$  species (409 ppm) yields data that can be used to obtain the equilibrium constant,

$$K = \frac{[\text{NO}^+][\text{NO}_3^-]}{[\text{N}_2\text{O}_4]}$$

We obtained values of 4.6M and 4.5M for K in 15% and 18%  $\text{N}_2\text{O}_4$  solutions. A  $^{14}\text{N}$  experiment on red fuming  $\text{HNO}_3$  revealed two NMR peaks. One is presumably  $\text{N}_2\text{O}_4$  (379 ppm vs ext.  $\text{NO}_3^-$ ) and the other a combined resonance for  $\text{NO}_3^-$ ,  $\text{NO}^+$ , and  $\text{HNO}_3$  (322 ppm). An equilibrium constant of  $K = 4.1\text{M}$  was determined in this case.

The transport of  $\text{HNO}_3$  and  $\text{H}_2\text{O}$  during electrolysis of  $\text{N}_2\text{O}_4$  is of interest in our laboratory. Data is available for  $^{18}\text{O}$  exchange in 40 to 62 wt %  $\text{HNO}_3$  but not in the concentration region, 90 wt %, of interest here. An attempt was made to measure the chemical exchange rate between  $\text{HNO}_3$  and  $\text{H}_2\text{O}$  in 93 wt %  $\text{HNO}_3$  by adding  $^{17}\text{O}$  enriched  $\text{H}_2\text{O}$  to anhydrous  $\text{HNO}_3$ . A constant distribution of  $^{17}\text{O}$  was observed during the entire experiment, 18 hrs, and found to be equal to the



expected ratio for complete isotopic exchange. The exchange rate is faster than the shortest time used to obtain our first NMR spectrum, ~ 15 minutes.

Table 1. NMR parameters for  $^{17}\text{O}$  in  $\text{HNO}_3/\text{H}_2\text{O}$  solutions.

Sample	Chemical Shift	
	water (ppm)	$\text{HNO}_3$ (ppm)
Bulk $\text{H}_2\text{O}$	0	--
3.1M $\text{HNO}_3$	3.3	413.5
10M $\text{HNO}_3$	9.0	411.0
21.8M $\text{HNO}_3$	2.1	409.6
Anhydrous $\text{HNO}_3$	-- *	407.9

\*Anhydrous  $\text{HNO}_3$  contains 0.4 wt %  $\text{H}_2\text{O}$ . We did not detect this water.

Sincerely,

  
James A. Happe

1448R  
JAH:jer

TITLE:  $^{17}\text{O}$  and  $^{14}\text{N}$  NMR Experiments on Nitric Acid Systems at 4.7T

Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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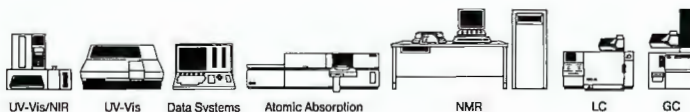
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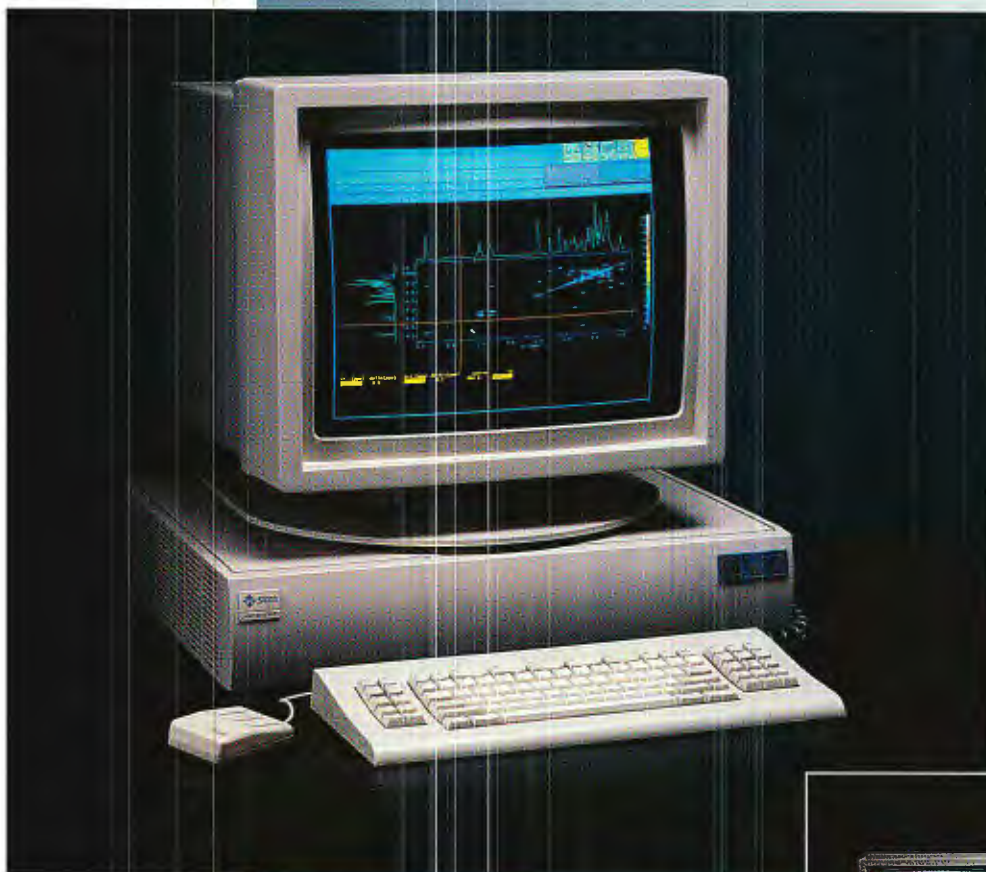


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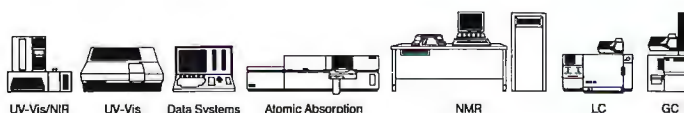
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FACULTAD DE CIENCIAS EXACTAS Y NATURALES

Buenos Aires, July 23, 1987  
(Received 20 August 1987)

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

An Intuitive, Though Rigorous, Analysis  
of Spin-Spin Coupling Constants

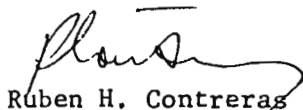
Dear Professor Shapiro,

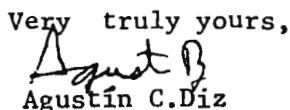
During the last few years we developed several methods to study different electronic contributions to spin-spin coupling constants. Briefly, they are the PRMO (Partially Restricted Molecular Orbitals) approach both in the FPT/1/ and SCPT /2/ versions, and the IPPP (Inner Projections of the Polarization Propagator) method /3,4/. The last one proved to be very useful to calculate contributions from different molecular fragments and is now available from an international distribution center /5/. Those molecular fragments are defined through a localization procedure by means of unitary transformations applied separately to occupied and vacant canonical orbitals. The IPPP method is particularly useful for calculating: i) sigma- and pi-transmitted components, ii) through space components and iii) components transmitted through different pathways in multicyclic compounds /6/. The analysis can be performed on the Fermi contact (FC), paramagnetic spin-orbital (PSO) and spin-dipolar (SD) contributions. Lately /7/, the IPPP method was modified in such a way that a molecular fragment component can be decomposed in contributions which originate in localized molecular orbitals that represent bonds, antibonds and lone-pairs. Now we wish to report that this last approach has been successfully extended to total couplings to write:

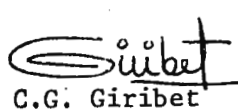
$$J(NN') = \sum_{i,j}^{i,j:\text{occup.}} \sum_{a,b}^{a,b:\text{unocc.}} (J_{ia,jb}^{\text{FC}}(NN') + J_{ia,jb}^{\text{PSO}}(NN') + J_{ia,jb}^{\text{SD}}(NN'))$$

where it should be stressed that  $i,j$  are localized occupied molecular orbitals that represent bonds or lone-pairs, and  $a,b$  are vacant localized molecular orbitals that represent antibonding orbitals. Results with this new approach, which we call CLOPP (Contributions from Localized Orbitals within the Polarization Propagator approach) will soon be published.

Please, credit this contribution to Prof. Valdemar J. Kowalewski's subscription.

  
Ruben H. Contreras

Very truly yours,  
  
Agustín C. Diz

  
C.G. Giribet

  
Martín Ruiz de Azúa

- 1) A.R. Engelmann, R.H. Contreras and J.C. Facelli, Theoret. Chim. Acta 59, 17 (1981).
- 2) A.R. Engelmann, G.E. Scuseria and R.H. Contreras, J. Magn. Reson. 50, 21 (1982).
- 3) A.R. Engelmann and R.H. Contreras, Int. J. Quantum Chem. 23, 1033 (1983).
- 4) M.A. Natiello and R.H. Contreras, Chem Phys. Lett. 104, 568 (1984).
- 5) A.R. Engelmann, M.A. Natiello, G.E. Scuseria and R.H. Contreras, Comp. Phys. Comm. 39, 409 (1986).
- 6) R.H. Contreras and G.E. Scuseria, Org. Magn. Reson. 22, 411 (1984).
- 7) M.C. Ruiz de Azúa, A.C. Diz, C.G. Giribet, R.H. Contreras and I.D. Rae, Int J Quantum Chem. S20, 585 (1986).



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Department of Physical Chemistry  
Professor Peter Stilbs

Date

Stockholm, August 6, 1987  
(Received 14 August 1987)

Professor B L Shapiro  
Department of Chemistry  
College Station  
Texas 77843-3255

U S A

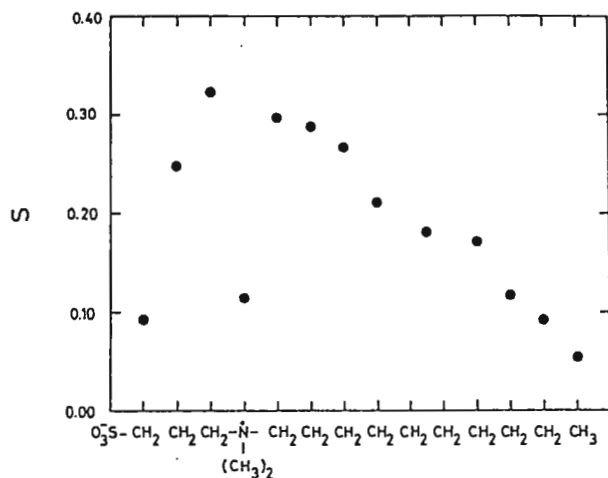
"Order parameters of micellized zwittergents"

Dear Barry,

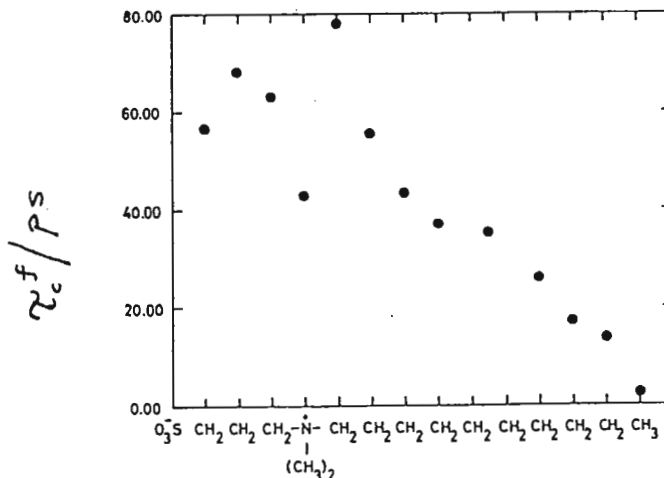
Thank you for your reminder. We just moved back to our remodelled building which appears to be relatively well designed. Most goods is still boxed and we do not hope for a much better time constant than  $2 \text{ year}^{-1}$  for asymptotically getting labs, spectrometers and everything else in order. On the other hand, we have been funded for a computer system and a new supercon magnet to upgrade our MSL-90. Most likely I will also order one SpecStation from New Methods Research very soon. I have also bought a used FX-100 from Stockholm University. We hope for a well-equipped and well-working lab a year from now.

As for science, we have not achieved very much during this past year in our temporary quarters. However, my students in Uppsala, Mikael Jansson and Li Pouyong and myself have done some further "two-step" spin relaxation work (1-2) on micellar systems, which may be of interest to some of your readers. Zwitterionic, micellized surfactants of the type  $\text{CH}_3-(\text{CH}_2)_n-\text{N}^+(\text{CH}_3)_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{SO}_3^-$  exhibit interesting order parameter and local reorientation profiles (Figs. 1 and 2). Both curves indicate that the dimethylamino group is located at the micellar surface in a relatively constrained chain conformation. The work will soon appear in J. Phys. Chem.

- 1) B. Halle and H. Wennerström, J. Chem. Phys. 75 (1981) 1928
- 2) H. Walderhaug, O. Söderman and P. Stilbs, J. Phys. Chem. 88 (1984) 1955.



The order parameter, obtained from the two-step model analysis of  $^{13}\text{C}$  relaxation and NOE data, of 0.36M DAPS at 25 °C as a function of carbon position in the surfactant chain.



The fast correlation times, obtained from the two-step model analysis of  $^{13}\text{C}$  relaxation and NOE data, of 0.36M DAPS at 25 °C as a function of carbon position in the surfactant chain.

Yours sincerely

*Peter Stilbs*

Peter Stilbs

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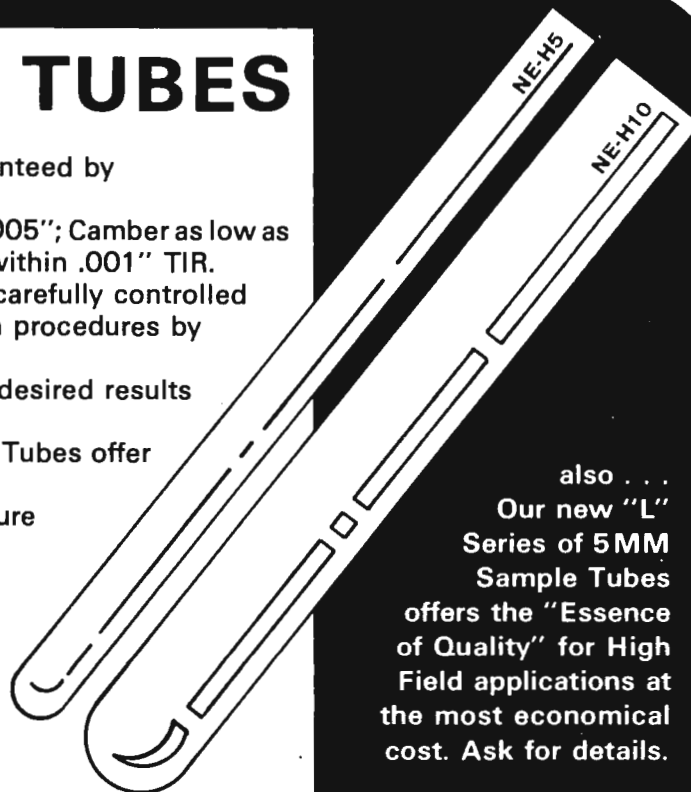
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 Dipl. Chem. Michael Grzonka and Prof. Gerhard Hägele  
 20.07.1987

(Received 7 August 1987)

Dissociation and Complex Formation  
Equilibria of Multibasic Acids

Dear Prof. Shapiro!

Summer term was busy - so we reply rather late to your reminder. We concentrated our recent interests towards dissociation and complex formation equilibria of multibasic acids, looking into classical analytical methods and NMR studies of phosphonic and phosphinic acids. We wished to obtain characteristic correlations between chemical shifts or coupling constants (e. g.  $\delta_P$ ,  $J_{PP}$ ) and various parameters (e.g. pH, degree of titration  $\tau$ , temperature) and to present our measurements from a series of single experiments in an appropriate form of display. In practice, after having acquired all experimental data, a heap of papers on a desk results, each paper holding one spectrum only at a certain value of the parameter under investigation. Therefore looking for correlations in complex situations is rather difficult. A few weeks ago we found a more convincing way of presenting our data. Since 2D-NMR has solved the same kind of problem a few years ago we called it 'pseudo-2D-NMR'. The procedure listed below is a useful tool for the investigation of 1D-spectra, showing as examples the variation of  $\delta_P$  for titrations of phosphoric acid and 1-phenyl-ethane-1,2,2-tris-(P-methylphosphinic) acid with suitable bases.

Essentially the FID's of our 1D-spectra are condensed to a single 2D-file by a short microprogram on our Bruker AM200. Transforming this data in the F2-domain only yields a file containing all the 1D-spectra, but stored in 2D manner. Subsequently all conventional 2D utility routines may be applied to this file yielding the plots wanted as shown in fig. 1 and 2. In our case especially the contour plots proved to be very helpful for the investigation of the phosphorus chemical shift during a titration, even in more complicated situations as shown in fig. 4.

Most of our work is dedicated to inspect correlations between  $\tau$ , the degree of titration, and the chemical shift  $\delta_P$  as shown in figures below. For internal use we named this technique  $\tau, \delta$ -COSY, which will be helpful for quite a variety of analytical studies.

Yours sincerely

*M. Grzonka*  
 Michael Grzonka

*G. Hägele*  
 Gerhard Hägele

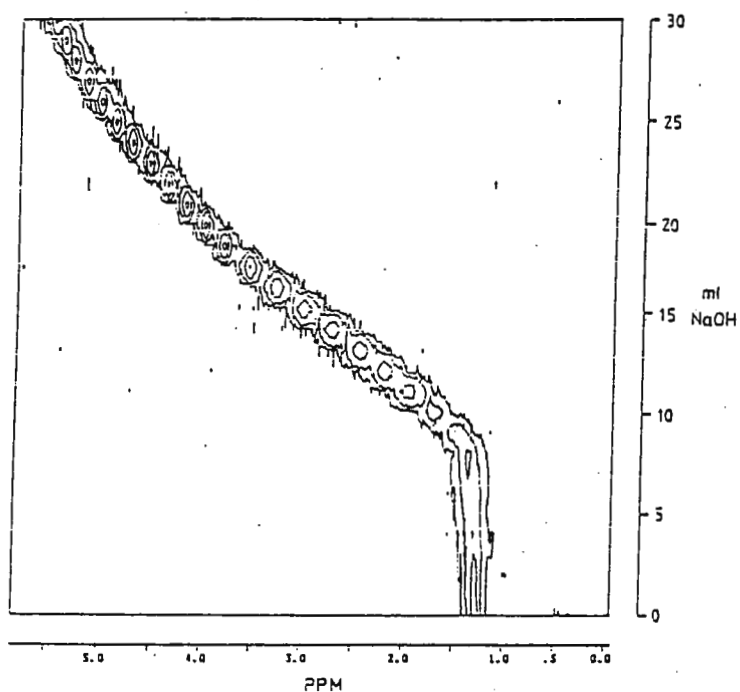
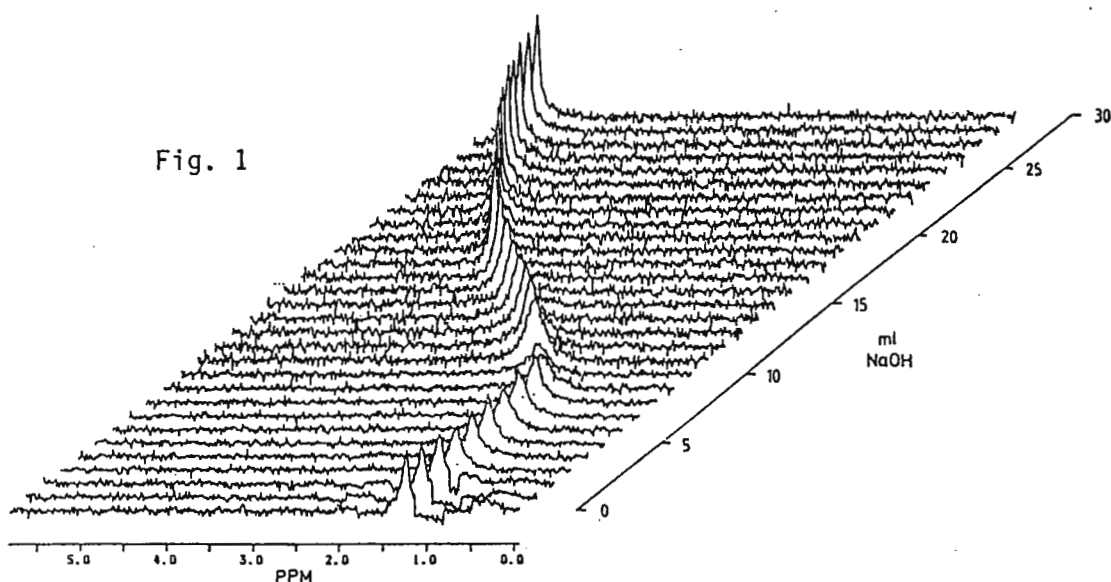
Title of contribution: "Pseudo-2D-NMR"

Procedure:

- 1) Put 1D-FID's into files having identical names but differing in extension numbers: e.g. SPEC.001, SPEC.002, ..., SPEC.013.
- 2) Set the number of experiments NE to the current number of files you want to access (e.g. 13)
- 3) Start the following microprogram:
 

1 ZE,	2 RF #1.001,	3 RE #1,	4 WR #2,
5 IF #2,	6 IF #1,	7 IN=3,	8 EXIT.

 Filename #1 is the name of the series of 1D FID's, filename #2 is the name of the .SER file to be established.
- 4) Set MC2 to 'W' and WDW2 to 'G'; set LB to an appropriate value if line broadening is required; set NDO to '1'.
- 5) Setup the 2D-file with: ST2D <name>.SER.  
Make sure that SI1 becomes equal to the next higher power of 2 after NE multiplied by 2. (e.g.: NE=13 ==> SI1=16\*2 = 32).
- 6) Fourier transform in F2-domain with the command XF2.



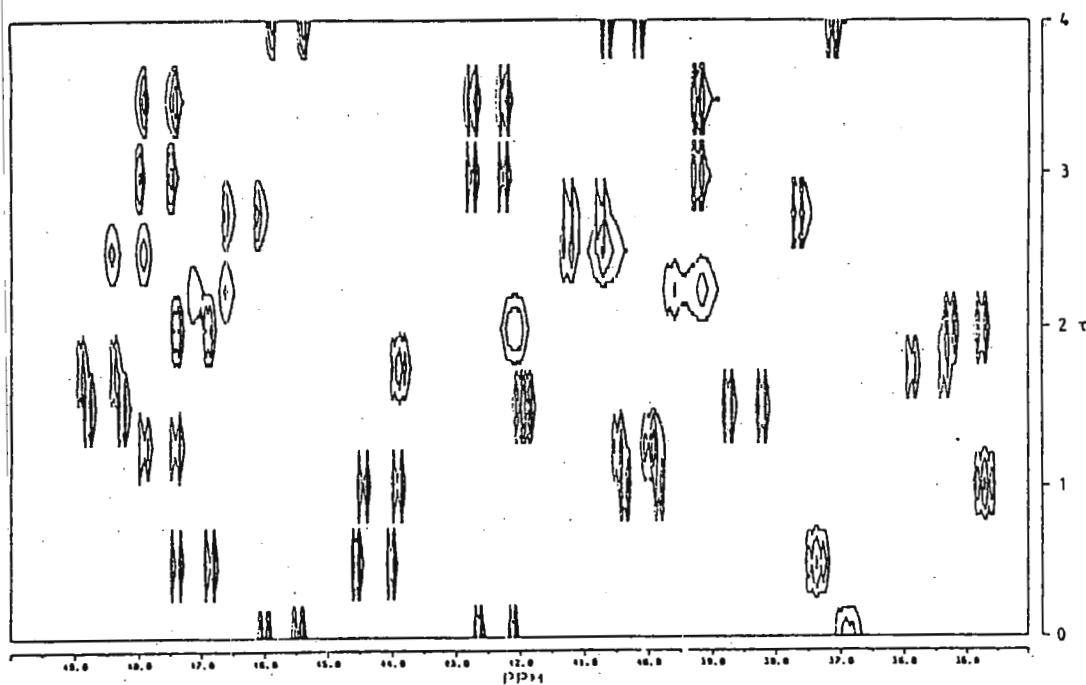
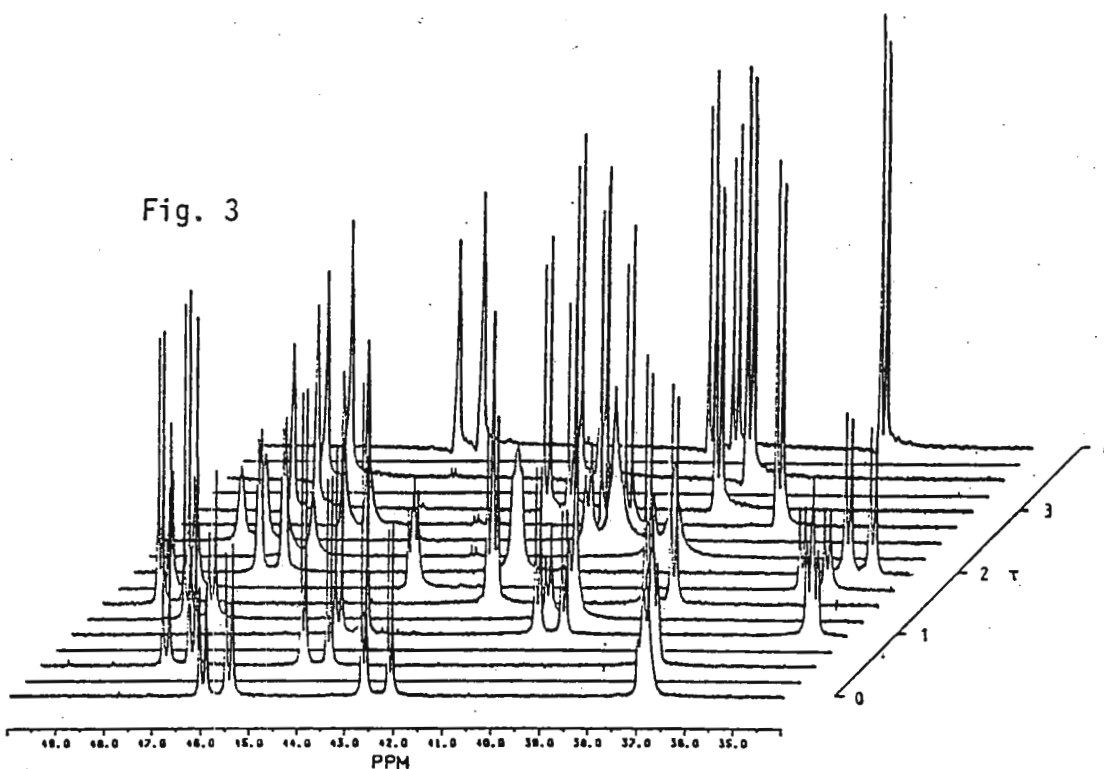


Fig. 1: Titration of 0.058 M phosphoric acid vs. 1.02 M NaOH

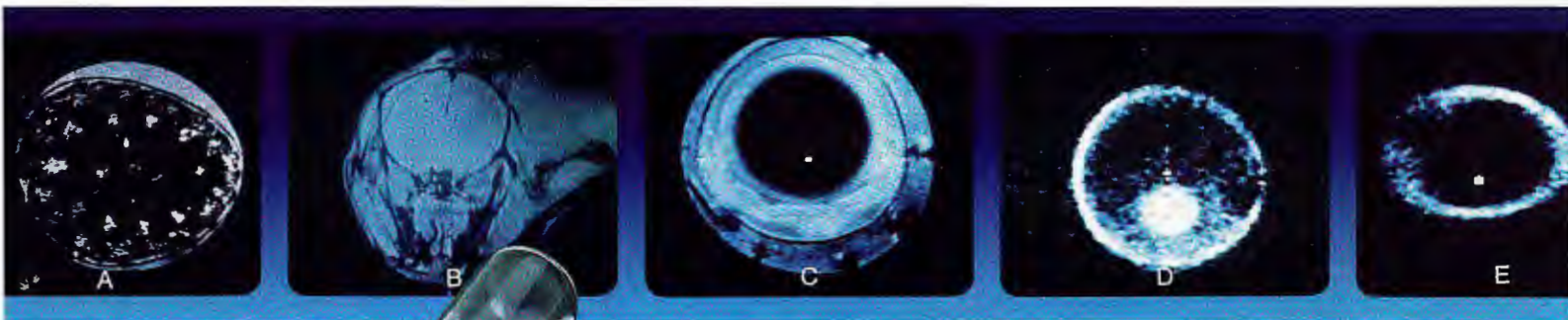
Fig. 2: as figure 1, but contour plot

Fig. 3: 0.1 M 1-phenyl-ethane-1,2,2-tris-(P-methylphosphinic) acid titrated with 1 M KOH/D<sub>2</sub>O

Fig. 4: as figure 3, contour plot (above)



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*Fig. A: Cross sectional image of a philodendron stem. Resolution  $19\mu \times 19\mu \times 300\mu$ .*

*Fig. B: Cross sectional image of a mouse brain tumor. Resolution  $100\mu \times 100\mu \times 500\mu$ .*

*Fig. C: A cross sectional image of a mouse eye, 3 mm in diameter. Resolution  $20\mu \times 20\mu \times 250\mu$ .*

*Fig. D: Image of an ovum from laevis (frog egg). Resolution  $10\mu \times 10\mu \times 250\mu$ .*

*Fig. E: Diffusion of water through a piece of nylon. Resolution  $50\mu \times 50\mu \times 1000\mu$ .*

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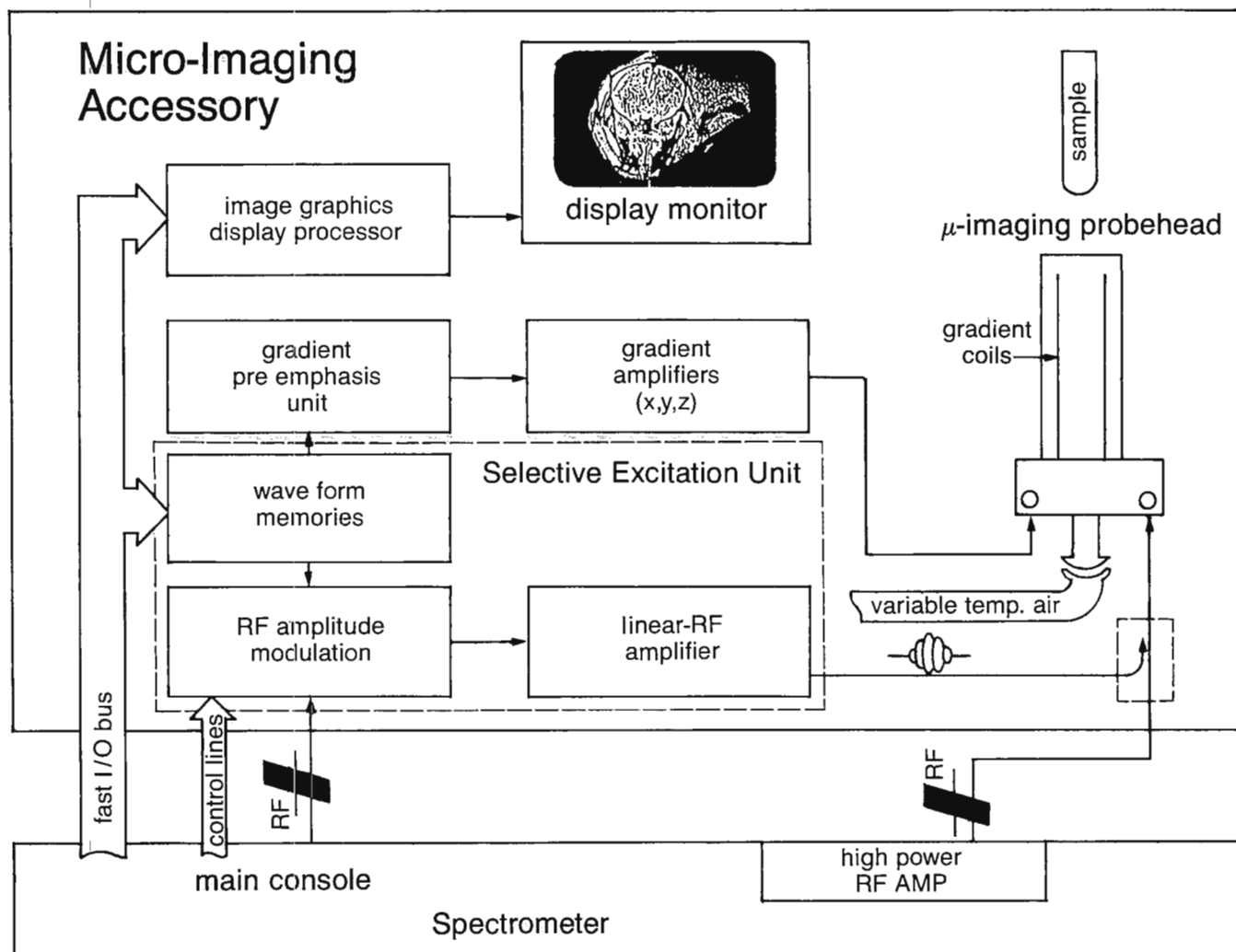
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DEPARTMENT OF PHYSICAL CHEMISTRY  
UNIVERSITY OF CAMBRIDGELENSFIELD ROAD  
CAMBRIDGE  
CB2 1EP

29 July 1987

Professor Bernard L. Shapiro  
Department of Chemistry  
Texas A. and M. University  
College Station  
Texas  
USA

Dear Barry

**THE EUROPEAN EXPERIMENTAL NMR CONFERENCE (1988)**

Next year the 9th EENC meeting will be held in Bad Aussee, a scenic area in the centre of Austria. The Conference will begin with a welcome mixer in the evening of Monday May 16th and will close on Friday May 20th, at noon. Lectures, posters and an instrument exhibition will be held in the Kurhaus, and participants will be housed in the nearby Hotel Post. The scientific topics will include biochemical NMR, high resolution solid-state NMR, two-dimensional spectroscopy, studies of motion in the solid state, stochastic excitation, imaging and in vivo NMR, computer networking and computer-aided NMR. The emphasis will be on new experimental techniques rather than applications.

Registration forms and further details can be obtained from the local organizer of the 9th EENC,

Professor H. Sterk  
Karl-Franzens-Universität Graz  
Institut für Organische Chemie  
Heinrichstrasse 28  
A-8010 Graz  
Austria.

Connoisseurs will remember recent European ENC meetings in Super Nendaz in Switzerland, Altavilla Milicia in Sicily and Spa in Belgium.

Kindest regards,



RAY FREEMAN



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Berkeley, California 94720

08/06/87

(Received 10 August 1987)

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

Guidelines for Delays in Long-Range CH Correlation Experiments:

Dear Prof. Shapiro:

Long-range CH correlation experiments are now routine techniques (at least in some laboratories) for spectral peak assignment and structure elucidation. Use of the conventional heteronuclear chemical shift correlation sequence [1] optimized

H:  $90^\circ - t_1/2 - -t_1/2 - \Delta_1 - 90^\circ - \Delta_2 - \text{BB}$   
C:  $180^\circ \quad 90^\circ \quad \text{Acq.}(t_2)$  [1]

for long-range magnetization transfer has the major drawback of intensity modulations due to direct bond couplings. Martin *et al.*<sup>1,2</sup> introduced a BIRD sequence midway through the refocusing delay ( $\Delta_2$ ) as in [2] (where  $\tau = 1/2 \cdot ^1J$ ) which

H:  $90^\circ - t_1/2 - -t_1/2 - \Delta_1 - 90^\circ - -90^\circ - \tau - 180^\circ - \tau - 90^\circ - -\text{BB}$   
C:  $180^\circ \quad 90^\circ - \Delta_2/2 - -180^\circ - \Delta_2/2 - -\text{Acq.}(t_2)$  [2]

effectively decouples one-bond modulation effects. Similar one-bond modulation decoupling during refocusing has been achieved by us<sup>3</sup> and others<sup>4,5</sup> in modifications of the COLOC sequence.

However, modulation of a long-range cross peak intensity due to other protons long-range coupled to the same carbon still persists. The response intensity function (I) (after one-bond modulation decoupling) for a cross peak arising due to polarization transfer from 'n' equivalent long-range coupled protons can be expressed as:

$$I = n * [\sin(\pi J \Delta_1) * \sin(\pi J \Delta_2) * \{\cos(\pi J \Delta_2)\}^{n-1}] * \prod \cos(\pi J' \Delta_2)$$

where J is the long-range coupling constant under observation and J' is the "interfering" long-range coupling constant. Though not as severe as one-bond modulations these long-range modulations must still be taken into consideration in optimizing the  $\Delta_1$  and  $\Delta_2$  values. The response intensity (I) can be written as a product of two terms  $I_0$  and  $I'$  each one being a function of either J or J'.

$$I = I_0 * \prod I'$$

where

$$I_0 = n * [\sin(\pi J \Delta_1) * \sin(\pi J \Delta_2) * \{\cos(\pi J \Delta_2)\}^{n-1}]$$

and

$$I' = \cos(\pi J' \Delta_2)$$

Response intensity ( $I_0$ ) contours as a function of J and  $\Delta_1$  (a choice of  $\Delta_2 = 0.5 * \Delta_1$  is ideally suited for a variety of situations) for long-range cross peaks (using sequence [2] or its variance) are given in Figs. 1-3. Similarly, attenuation factor ( $I'$ ) contours as a function of J' and  $\Delta_1$  are given in Fig. 4. From an estimate of the long-range coupling constant under observation and other interfering long-range coupling constants one is able to choose the optimum delay values from these contour maps. Though these considerations are still qualitative and assume first-order couplings we find these contour maps useful even for systems with strong second-order coupling network.

Sincerely,

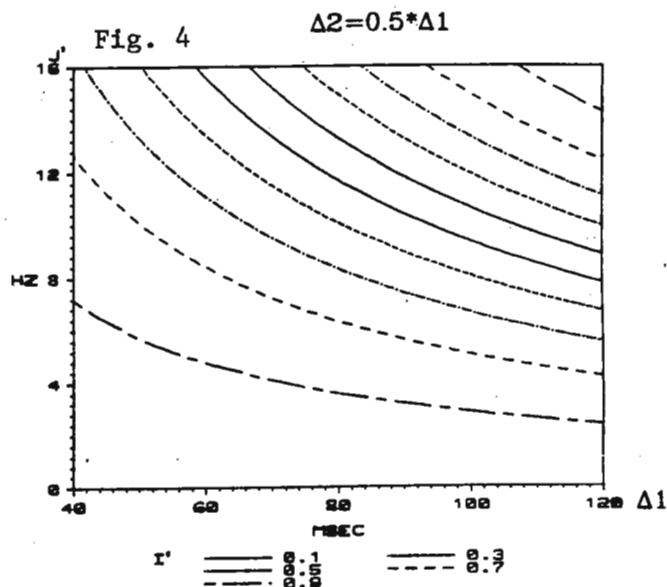
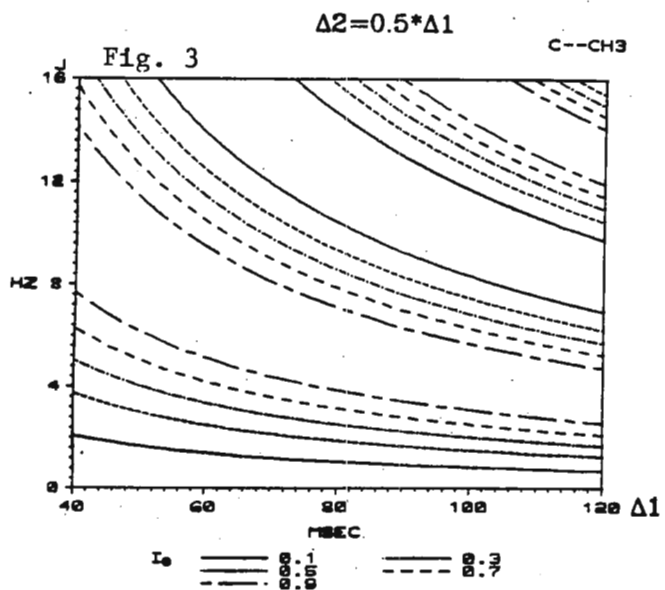
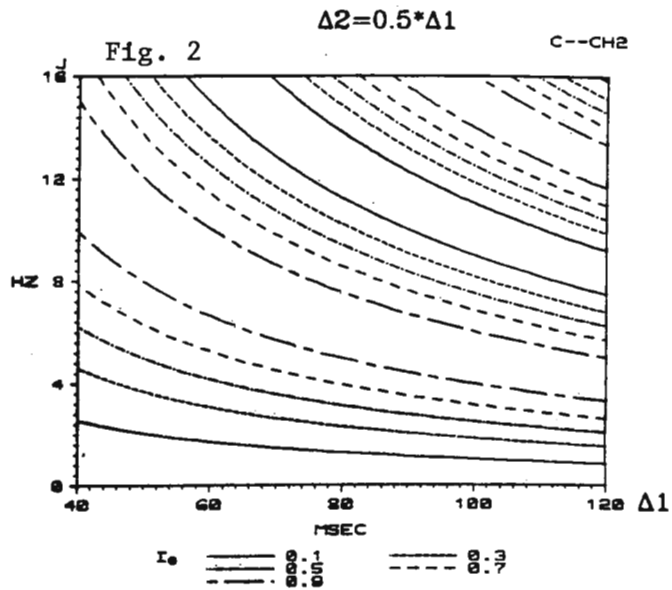
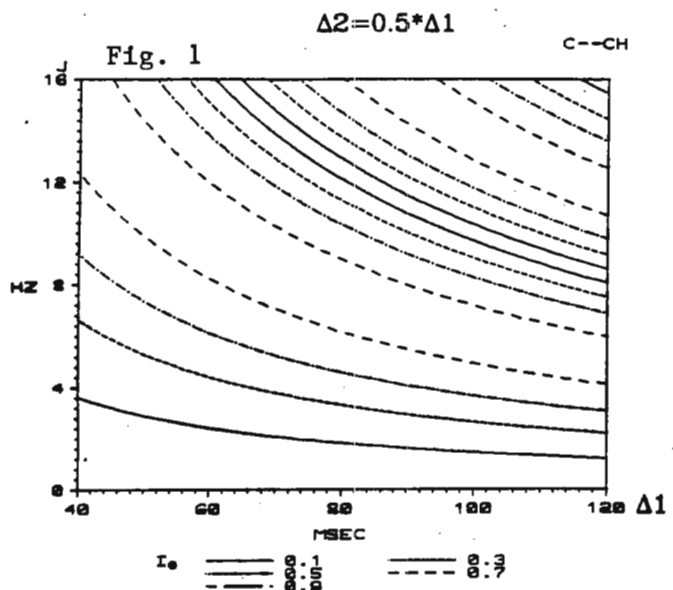
*V.V. Krishnamurthy*

V.V. Krishnamurthy  
NMR Specialist

P.S.: Please credit this contribution towards my account.

#### REFERENCES:

1. A. Zektzer, B.K. John, R.N. Castle and G.E. Martin, J. Magn. Reson., 72 556 (1987).
2. G.E. Martin and A. Zektzer, TAMU Newsletter, May, 1987.
3. V.V. Krishnamurthy and J.E. Casida, Magn. Reson. Chem., in press.
4. C. Bauer, R. Freeman and S. Wimperis, J. Magn. Reson., 58, 526 (1984).
5. W.F. Reynolds, D.W. Hughs, M. Perpich-Dumont and R.G. Enriques, J. Magn. Reson., 63 413 (1985).



Figs.1-3. Response intensity contours (in the absence of any modulation due to other couplings) as a function of  $J$  and  $\Delta_1$  values for a cross peak with polarization transfer from a methine proton (Fig.1), a set of methylene protons (Fig.2) and a set of methyl protons (Fig.3).

Fig.4. Attenuation factor contours calculated as a function of  $J'$  and  $\Delta_1$  values.



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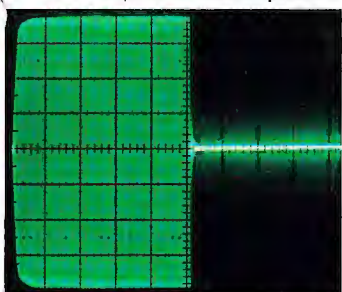
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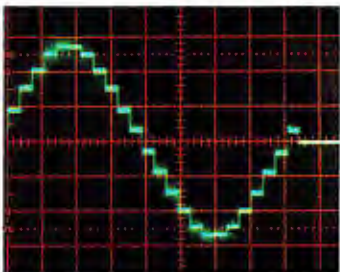
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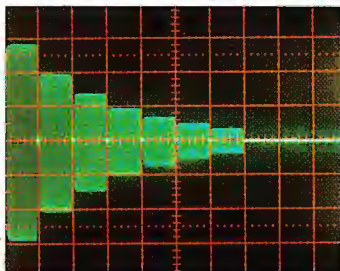
A 5 $\mu$ sec  $^1$ H observe pulse. ▾



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Shaped decoupler pulse. ►



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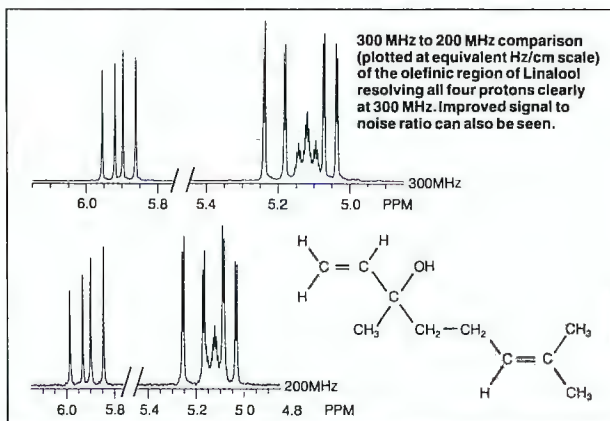
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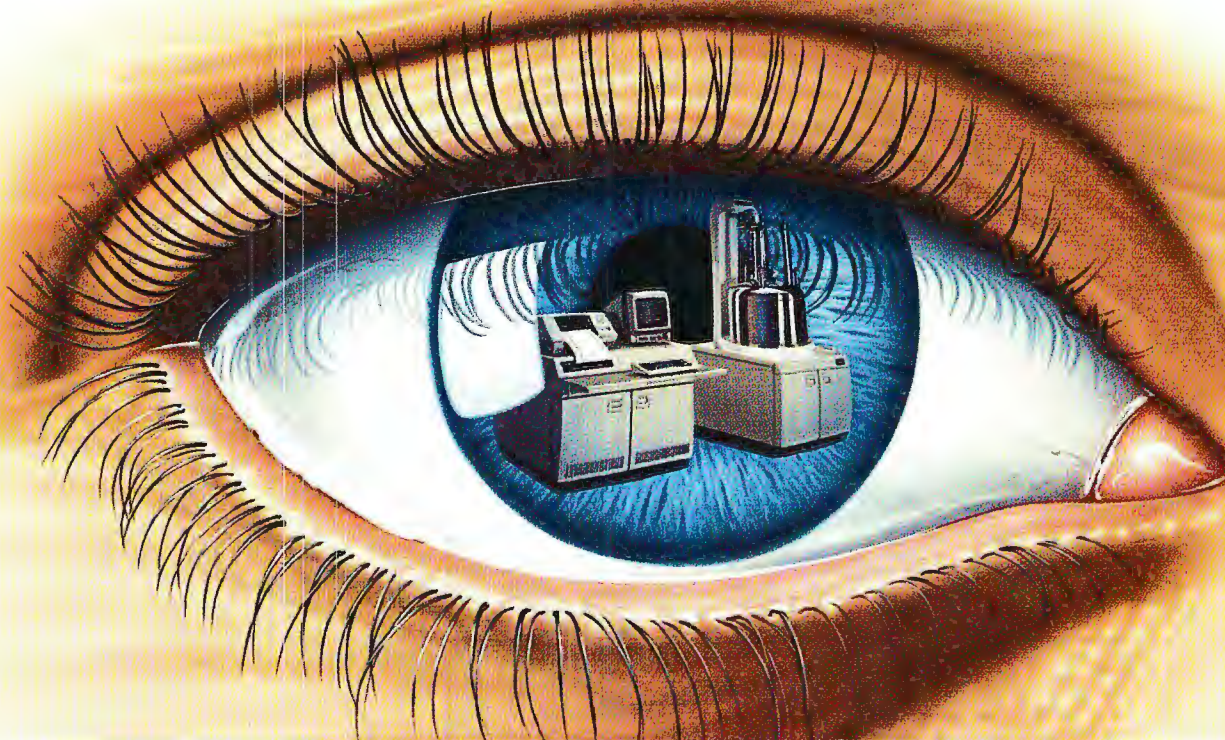
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University of California Service  
Veterans Administration Medical Center  
4150 Clement Street (11D)  
San Francisco, California 94121  
(415) 750-2146

August 12, 1987  
(Received 17 August 1987)

TAM Newsletter  
c/o Dr. Bernard L. Shapiro  
Department of Chemistry  
Texas A&M University  
College Station, Texas 77843

Dear Dr. Shapiro;

The Department of Radiology, University of California, San Francisco is seeking an Adjunct Assistant Professor to participate in NMR spectroscopy studies of animals and humans. Applicants should have a Ph.D. in Chemistry, Physics, Electrical Engineering, or related fields, and postdoctoral experience in the area of in vivo Nuclear Magnetic Resonance. Expertise in the areas of NMR localization techniques, imaging and chemical shift imaging, and RF engineering is required. A good understanding of the biochemistry of energy metabolism is also desirable.

The successful applicant will perform NMR studies of humans and animals, design and implement NMR methods to answer questions of clinical and biochemical interest, and process and interpret data. He or she will be expected to develop an independent research program and seek funding to support this research. This work will be done in collaboration with a large group scientists with interests in a number of areas related to in vivo NMR imaging and spectroscopy, under the general direction of Dr. Michael Weiner. The successful applicant will have generous access to a Philips Gyroscan spectrometer with a spectroscopy package, operating at 2 Tesla, a GE 2T 30 cm bore spectrometer, and a 7 T, 18 cm bore NMR system with imaging capability, as well as a variety of RF equipment and computing systems. Send curriculum vitae, an outline of proposed research, and addresses of three references to Dr. M.W. Weiner, Magnetic Resonance Laboratory (11D), Veterans Administration Medical Center, 4150 Clement Street, San Francisco, CA, 94121

Sincerely,

MICHAEL W. WEINER, M.D.  
Associate Professor of Medicine and Radiology

MWW/let



Department of Chemistry  
University of Denver  
Denver, CO 80208

August 9, 1987 (Received 17 August 1987)

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

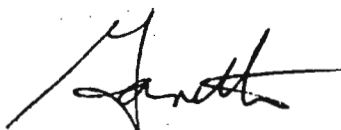
Dear Barry:

$^1\text{H}$  NMR spectra of spin-labeled complexes of Ni(II)

As part of our on-going studies of intramolecular interactions between non-equivalent paramagnetic centers, we have obtained  $^1\text{H}$  NMR spectra of spin-labeled complexes of Ni(II). We wanted to determine whether the isotropic shifts due to the Ni(II) unpaired electrons and the nitroxyl unpaired electrons were additive. The electron spin relaxation rate of nitroxyl radicals is too slow to obtain well-resolved NMR spectra of them in dilute solutions. High concentrations ( $> 1\text{ M}$ ) are usually used such that collisions cause increased relaxation rates and improved resolution of the NMR spectra. Our Ni(II) complexes with ligands that contain nitroxyl radicals are not sufficiently soluble to work at these concentrations. However, the paramagnetic Ni(II) provides an efficient relaxation mechanism for the nitroxyl radical and the spectra of the Ni(II) complexes that we obtained at  $0.1\text{ M}$  were as well resolved as spectra of nitroxyl radicals alone at  $1.0\text{ M}$ . A sample spectrum is shown in the accompanying figure. This efficacy of metal relaxation was first observed by Sagdeev, et al., JMR 9, 13 (1973), but does not appear to have been exploited by others.

We compared the isotropic shifts for a Ni(II) complex of a diamagnetic ligand and a Ni(II) complex of a nitroxyl radical. The isotropic shifts were calculated as the difference between chemical shifts for 4-coordinate complexes of diamagnetic Ni(II) and six-coordinate 2,2'-bipyridine (bpy) adducts of paramagnetic Ni(II). The data indicate that the contributions to the isotropic shifts of the protons from the two paramagnetic centers are additive within experimental error (which is fairly large for these broad lines). Additional examples, for other spin-labeled ligands, will be submitted for publication shortly.

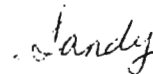
Sincerely,



Gareth R. Eaton

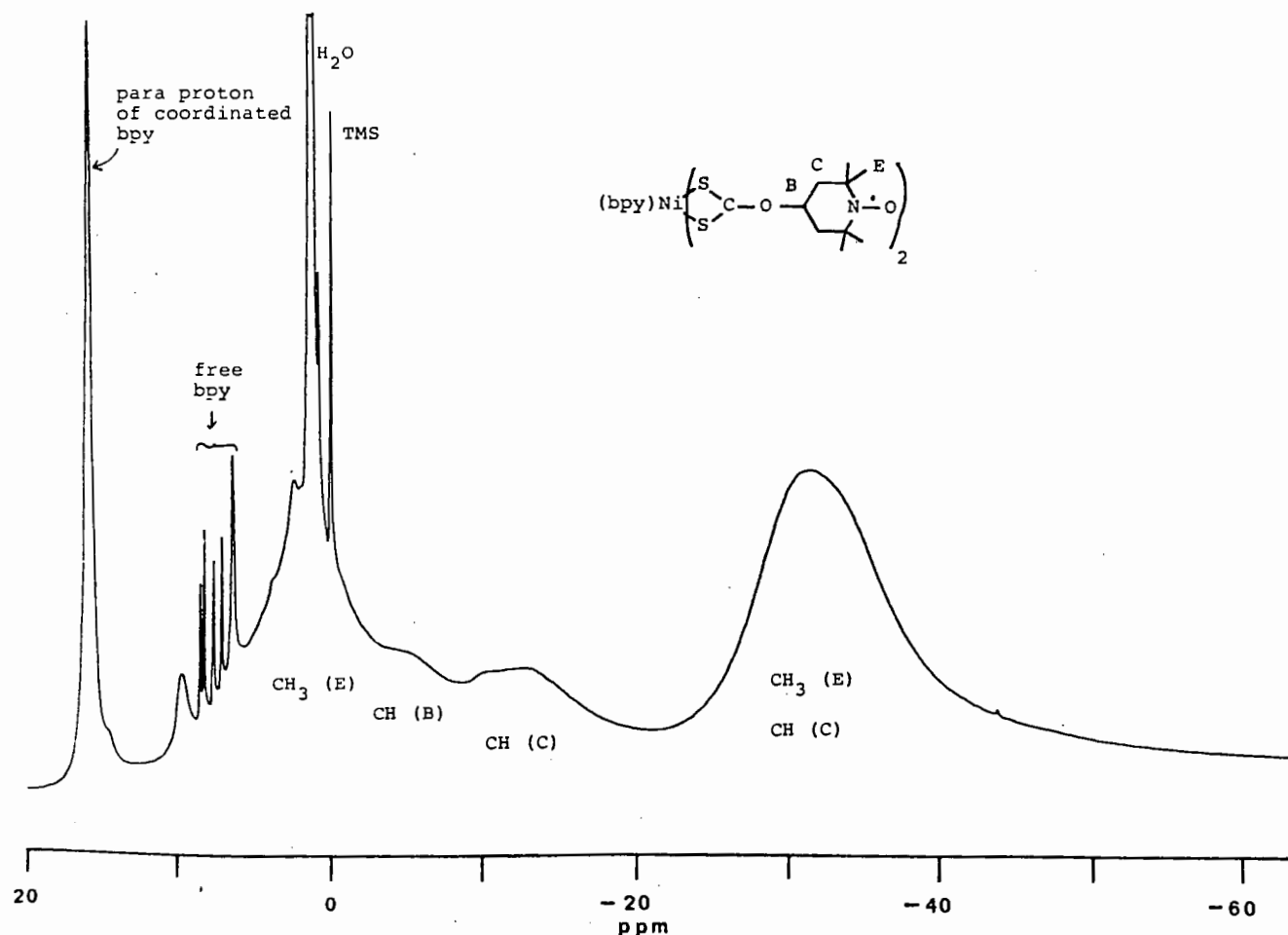


Scott Sheppard



Sandra S. Eaton





The Eastman Chemicals Division of Eastman Kodak Company in Kingsport, Tennessee, has an opening for a NMR specialist in their Research Laboratories. Candidates must have an outstanding knowledge of the theory of NMR, its application to the characterization of organic molecules, and practical experience operating the equipment. Extensive knowledge of proton and carbon NMR techniques, both 1D and 2D, is required. It would also be highly desirable for the candidate to have experience applying NMR to the characterization of polymers and/or other macromolecules. A strong background in physical chemistry is also desired. The applicant's duties will include responsibility for maintaining a JEOL GX-400 NMR spectrometer, interpreting spectra obtained from a variety of polymer intermediates, participating in problem-solving teams, and conducting a research program to elucidate the structure of polymers. Interested candidates should send resumes to: Betty W. DeVinney, Personnel Department, Tennessee Eastman Company, P. O. Box 1975, Kingsport, Tennessee 37662



August 7, 1987  
(Received 13 August 1987)

Professor B. L. Shapiro  
Department of Chemistry  
Texas AM University  
College Station, TX 77843

Dear Professor Shapiro:

Subject: Talaris Laser Printer Plotting of FTNMR Spectra

During our investigation of the usefulness of Dennis Hare's FTNMR software package for processing spectral data from our JEOL GX-series NMR spectrometers, we realized a need for each person to be able to plot data processed by FTNMR conveniently. Purchase of individual plotters for each user at each terminal was out of the question. To circumvent this problem, we developed FORTRAN software that plots the spectra on a Talaris Laser Printer. This program, TALARIS, plots spectral data files that have been created from FTNMR using the PM (Plot Mode) = 3 capability with DR (DRAW) or CP (Contour Plot). PM=3 creates a disk file (with the .PLT extension) containing the data previously displayed and includes notation to enable "move" and "draw" instructions for each data point in the file. Data input to TALARIS is from a data file created external to TALARIS so that plots for a large number of spectra can be requested at one time without additional input from the scientist. There is sufficient flexibility to allow plots in landscape or portrait modes of one or more spectra per page with any combination of spectra per page being requested during initial data input. 1D and 2D data sets can be plotted with TALARIS. This is a good example of the flexibility offered by FTNMR in providing data in a format compatible with our needs. Also we want to thank Dennis for working with us to decipher his .PLT file format.

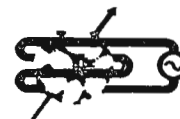
The Eastman Chemicals Division of Eastman Kodak Company in Kingsport, Tennessee, has an opening for a NMR specialist in their Research Laboratories. Please see the position available notice elsewhere in this issue of the NMR Newsletter.

Sincerely yours,

D. W. Lowman  
Senior Research Chemist  
Research Laboratories  
P. O. Box 1972

Enclosure/der/TR41541

# NMR CONCEPTS



## 1987-1988 COURSE SCHEDULE

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### ELECTRONICS FOR NMR TECHNICIANS

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### INTERPRETATION OF NMR SPECTRA

Lichter & Traficante  
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6 Nov 87, Lab \_\_\_\_\_ URI/Rhode Island

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Maciel & Frye  
16-20 Nov 87 \_\_\_\_\_ Fort Collins CO  
18 Nov 87, Lab \_\_\_\_\_ Fort Collins CO  
21 Nov 87, Lab \_\_\_\_\_ Fort Collins CO

### INTRODUCTION OF SOLID STATE NMR

Maciel  
16-17 Nov 87 \_\_\_\_\_ Fort Collins CO

### QUANTUM MECHANICS OF SOLID STATE NMR

Maciel  
18 Nov 87 \_\_\_\_\_ Fort Collins CO

### ADV. TECH. & APPL. OF SOLID STATE NMR

Maciel  
19-20 Nov 87 \_\_\_\_\_ Fort Collins CO

### NMR CONCEPTS & OPERATING TECHNIQUES I

Traficante  
6-10 Dec 87 \_\_\_\_\_ \*WPCC/Rhode Island  
11 Dec 87, Lab \_\_\_\_\_ URI/Rhode Island

### IN-VIVO & IN-VITRO BIOLOGICAL NMR

Ackerman, Balaban & Satterlee  
11-15 Jan 88 \_\_\_\_\_ St. Louis MO  
16 Jan 88, Lab \_\_\_\_\_ Wash. Univ. MO

### 2D NMR FOR ORGANIC CHEMISTS

Rodger & Traficante  
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### 2D NMR FOR SPECTROSCOPISTS

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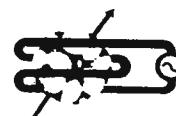
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## History of the series:

NMR Concepts is a non-profit, tax exempt school. It offered its first course in December of 1980 on the basic fundamentals of Nuclear Magnetic Resonance and discussed the physical concepts of NMR, beginning with signals generated in the rotating frame, carried through block diagrams of a spectrometer console, into the computer and finally represented in terms of a spectrum. The course included spectrometer operation, the Fourier transform, apodization and data treatment, relaxation measurements, and NOE's. The school has grown rapidly and now offers 28 courses in spectroscopy, ranging from basic fundamentals to state-of-the-art techniques. The lecturers come from the US, Canada, England, and West Germany. All are pioneers in NMR and work at developing state-of-the-art techniques and instrumentation. The courses are high-quality, in-depth treatments of specialized topics, and were developed in direct response to expressed community needs. They are designed to prepare the attendee to enter into a specific area of spectroscopy.

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Indianapolis, Indiana 46285  
(317) 276-2000

August 6, 1987 (Received 10 August 1987)

Professor B. L. Shapiro  
Department of Chemistry  
Texas A & M University  
College Station, TX 77843-3255

Dear Barry:

## SOMETHING OF A SETBACK

Recently our IBM 9000 laboratory computer acquired a problem which we finally traced to the mother board. When we inquired about the possibility of repair, the estimate given us by IBM was higher than the price of an AT compatible! Accordingly we decided to "surplus" the 9000 and start over with hardware that someone other than ourselves had heard of ("You want to order floppy diskettes for an IBM *what?*"). At the moment the XT that usually resides on my desk is in the NMR lab trying to fill the role of the old 9000.

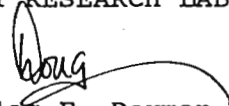
In some respects the XT is an ideal solution. For example, for the 9000 we had to write our own simple data base program; for the XT the major problem is deciding which of the many commercial systems to buy. There are also graphics programs available, and any number of expert system shells. Finally, there are more language compilers available for the "compatibles." I have taken advantage of this to teach myself PROLOG during the last few months.

But we have lost many useful 9000 programs, and we are slowly trying to recover lost ground. We have gotten the three programs incorporated into ARM (*cf.* TAMU, #309, p. 61, 1984) going on the XT, and we have made a beginning in the task of replacing REFSPEC (*ibid.*), a program designed to automate spectrum correlation and to draw the resulting correlation diagram. We have also, with Leo Joncas' (Bruker, Billerica, MA) help, established a KERMIT connection between the XT and at least one of the spectrometers. And we have *lots* of ideas...

But, we have little to report this time. As usual, we would be delighted to hear from other readers who are involved in similar struggles.

Sincerely,

LILLY RESEARCH LABORATORIES

  
Douglas E. Dorman, Ph.D.  
Research Scientist  
Physical Chemistry Research

## CENTRO DE INVESTIGACION DEL IPN

APARTADO POSTAL 14-740

MEXICO 14, D. F.

Telex: 017-72826

DEPARTAMENTO DE QUIMICA

August 14, 1987

(Received 20 August 1987)

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

Definitive assignment of the  $^{13}\text{C}$  NMR signals of indole

Dear Professor Shapiro:

In a recent review about the  $^{13}\text{C}$  NMR spectra of almost 300 indole derivatives having no substituent at the benzene ring (1), we were able to reassign some chemical shifts or to consider some assignments as doubtful. This situation highlights the need for careful experimentation that allows secure interpretations, since in many cases contradictory assignments are reported. This is particularly true for the C-4, C-5 and C-6 signals of indole, which appear in a narrow range of chemical shifts.

For indoles, some 67% of the reported data were measured from  $\text{CDCl}_3$  solutions, some 15% in  $\text{DMSO}-d_6$ , some 8% in mixture of these two solvents and only the remaining 10% in a variety of other solvents. Furthermore, many assignments were derived using the contradictory chemical shifts of parent indole (see Table) either in chloroform (2,8) or in dimethylsulfoxide (8,12) solutions as the model compound, and therefore for this molecule further evaluation, specially at high magnetic fields, seems desirable.

Since the  $^1\text{H}$  NMR chemical shifts of indole are solvent and concentration dependent (13) safe assignments of both the  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra in  $\text{CDCl}_3$  and in  $\text{DMSO}-d_6$  can be obtained from two-dimensional heteronuclear chemical shifts (HETCOR) contour plots combined with homonuclear double resonance experiments. Since the signal owing to C-7 is well defined (1) for most compounds as to appear in the 111-115 ppm region, direct assignment to H-7 follows from the two-dimensional experiments. This allows from the multiplicities to assign H-4, which upon homonuclear irradiation provides direct interpretation of the remaining benzene ring protons, and then the HETCOR allows the assignment of the carbon signals. The determination of HETCOR contour plots at different indole concentrations, revealed that although in  $\text{CDCl}_3$  solutions some  $^1\text{H}$  signals change in their chemical shift apparition order, their order do not changes in the  $^{13}\text{C}$  domain. For  $\text{DMSO}-d_6$  solutions no such changes occur at all, a situation which is understandable due to strong solvation.

It should also be noted that the values derived from the present study (Table) correspond to measurements at  $27^\circ\text{C}$  using 0.83M solutions on a XL-300GS system.

$^{13}\text{C}$  NMR Shifts of Indole

C-2	C-3	C-3a	C-4	C-5	C-6	C-7	C-7a		Ref
124.1	102.1	127.6	120.5	121.7	119.6	111.0	135.5	CDCl <sub>3</sub>	2
123.7	101.8	127.0	119.9	121.1	119.0	110.4	134.8	CDCl <sub>3</sub>	3
123.2	102.5	128.0	120.8	119.9	122.0	111.2	135.8	CDCl <sub>3</sub>	4
124.3	101.9	127.6	120.6	121.7	119.7	111.1	135.6	CDCl <sub>3</sub>	5
124.4	102.0	127.6	120.6	121.8	119.7	111.2	135.6	CDCl <sub>3</sub>	6
123.9	102.5	127.5	120.6	119.5	121.7	110.7	135.5	CDCl <sub>3</sub>	7
124.2	102.4	127.8	120.7	119.8	121.9	111.1	135.7	CDCl <sub>3</sub>	8
125.0	101.0	127.7	120.0	120.9	118.8	111.4	136.0	DMSO-d <sub>6</sub>	9
125.2	102.6	128.8	121.3	122.3	120.3	111.8	136.1	DMSO-d <sub>6</sub>	10
125.1	101.1	127.7	120.0	118.8	120.9	111.4	135.9	DMSO-d <sub>6</sub>	11
124.8	102.0	128.4	120.9	121.5	119.9	111.4	135.7	DMSO-d <sub>6</sub>	12
125.1	100.9	127.6	119.9	118.7	120.8	111.3	135.8	DMSO-d <sub>6</sub>	8

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M.S. Morales-Ríos

Sincerely yours


  
Pedro Joseph-Nathan

Varian / 611 Hansen Way / Palo Alto / California 94303 / U.S.A.

Tel. (415) 493-4000

Telex 34-8476

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



Dear Barry:

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Yours sincerely,

*Howard*

Howard Hill M/S D-317  
611 Hansen Way  
Palo Alto, CA 94303-0883

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# University of Durham

Department of Chemistry

Telex: 537351 DURLIB G

Science Laboratories, South Road, DURHAM,  
GREAT BRITAIN, DH1 3LE  
Telephone: Durham (091) 374 3121

*Professor of Chemistry:*

Robin K. Harris

4th August, 1987.

(Received 19 August 1987)

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

Dear Professor Shapiro,

## NOTATION AND RELATED BORING MATTERS

It cannot have escaped the notice of most NMR spectroscopists that some aspects of common practice in NMR make our subject a good (!) contender for a prize for the most ridiculous notation. Take "multinuclear NMR" for example. Don't people who use this phrase realise that the N in NMR stands for "nuclear"? Then there's the term "sweep width" - for an experiment in which no variable is swept these days. My pet hate is for the use of "high field" to mean, not work at 11.7 T and above, but rather "to low frequency" or "increased shielding". Of course, the words I dislike are of historic interest and once had a sensible meaning in terms of experimental practice, but that is so no longer.

Abbreviations/acronyms multiply at a great rate in NMR. Some are clever; others are absurd. I guess we need some way of easily identifying, for example, pulse sequences, but current usage is a jungle of confusion. Someone (not me!) should write a definitive dictionary of terms. It seems to me that one principle should be that shorter forms should be chosen rather than longer. For that reason I much prefer MAS to MASS. Actually, it appeared to me that MAR was best (Rotation rather than Spinning) because I believe it was actually coined first, but I've given up that battle - the big battalions of Americans have, as so often, overwhelmed the scientific community in general.

Symbols are another area where some sensible uniformity is desirable. I suppose all NMR spectroscopists are familiar with the confusion that sometimes occurs with  $\delta$  (chemical shift-positive frequency convention) and  $\sigma$  (shielding), though in my view there should be no difficulty provided the two symbols are always used with the appropriate meaning (the term "chemical shift" is itself somewhat ambiguous as to the meaning of sign). However,  $\delta$  is often used in tensor notation to mean anisotropy, e.g. in shielding (but with a different definition from  $\Delta\sigma$ ). Such a symbol  $\delta$  can clearly be

confused with the chemical shift scale  $\delta$ , so I propose use of a new symbol  $\beth$  (hebrew letter beth) for the anisotropy meaning. Incidentally, my friend Dr. A-R. Grimmer, from the Central Institute for Inorganic Chemistry in East Berlin, points out that the asymmetry parameter,  $\eta$ , also measures a form of anisotropy, so that it is preferable not to use that word for  $\delta$  (i.e.  $\beth$ ) or  $\Delta\sigma$ . He suggests the word axiality, which I believe is sensible. For quadrupolar interactions, the nuclear quadrupole coupling constant (in frequency units) has usually been written  $e^2q_{zz}Q/h$ , which is clumsy. The use of  $\chi$  for this quantity appears to be growing and has much to recommend it.

So here's my partial (in both senses) list of good and bad:

<u>Poor notation</u>	<u>Acceptable notation</u>
multinuclear NMR	multinuclear magnetic resonance or multi-NMR
sweep width	spectral width
number of scans	number of transients
pulse length	pulse duration
high/low field	low/high frequency
MASS	MAS
$\delta$ (for anisotropy)	$\beth$
$e^2q_{zz}Q/h$	$\chi$
anisotropy (for $\Delta\sigma$ or $\beth$ )	axiality

Additions to this list, comments, and further (polite) suggestions would be welcomed. In particular, can anyone suggest a better phrase than the ambiguous "multipulse sequence" for pulse trains interspersed with single-point acquisitions as in the WAHUA and MREV-8 situations? IUPAC is now beginning to take a strong interest in NMR notation and practice (particularly as to the hoary old subject of referencing) - more details will appear in a later TAMU NMR letter - so it is timely for these questions to be discussed.

As to referencing, many problems would be avoided if we always obtained spectra with spinning at the magic angle, since that would appear to eliminate effects from differences in isotropic bulk susceptibility. So here's a tongue-in-cheek suggestion for the spectrometer manufacturers: why not make solution-state systems with the usual slow spinning ( $\sim 10$ -20 or perhaps a few hundred Hz) but about the magic angle rather than z or y? While they're about it, they could make first-order shim coils which are relevant directly to the magic angle and thus make life easier for the solid-state NMR spectroscopist.

Does this letter count as a "subscription"? With reluctance - BLS

Best wishes,

Yours sincerely,

*Robin*

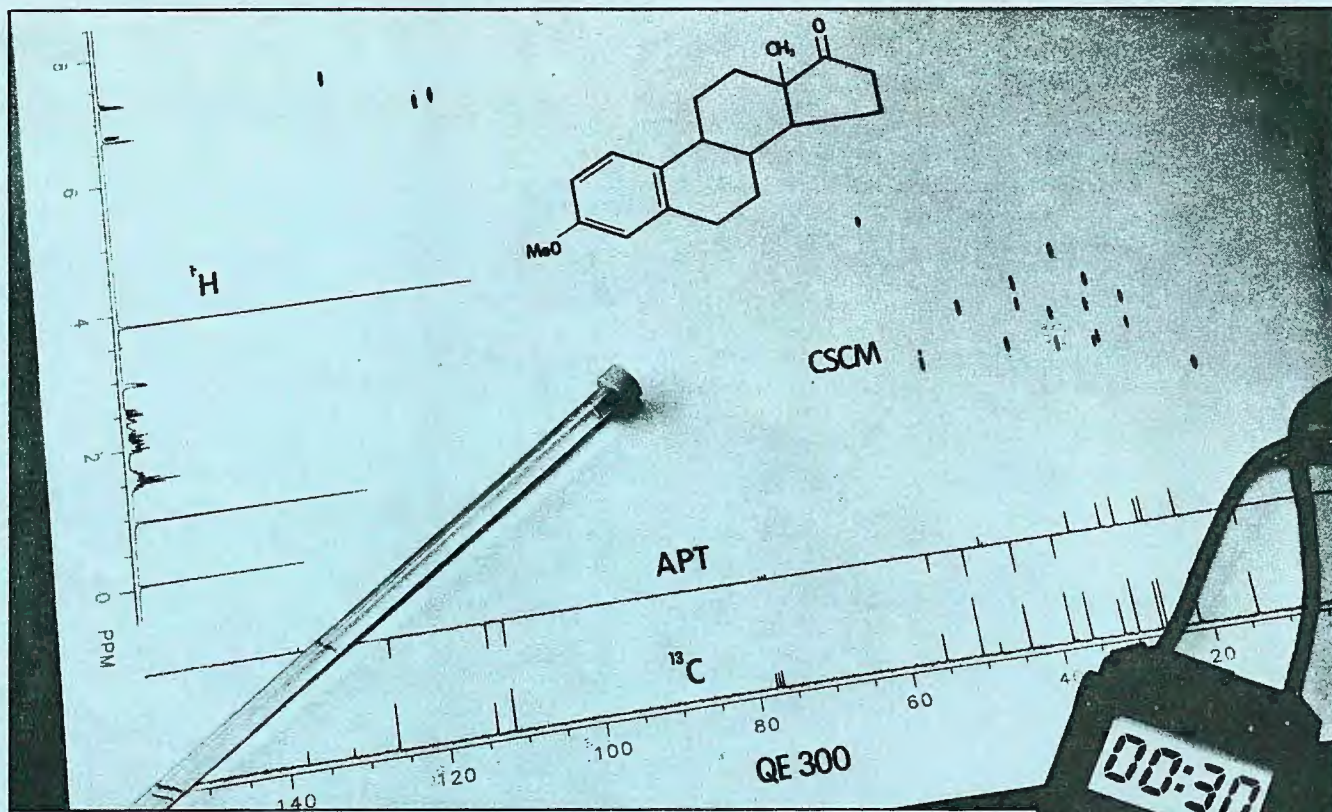
R.K. Harris

#### TAMU NMR NEWSLETTER SUBSCRIPTIONS FOR 1987-1988

By the time you receive this Newsletter, you should have received and processed your invoice for the 1987-1988 subscription year. If you have not received an invoice, please let me know immediately, as the October 1987 issue will not be sent to unpaid subscribers.

B.L. Shapiro





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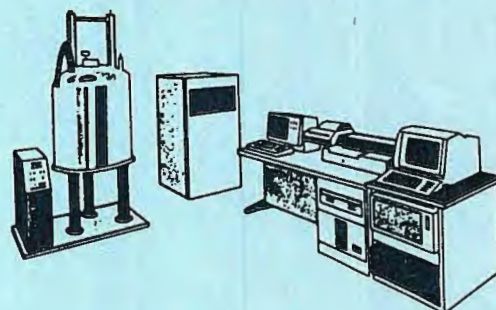
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