Joseph B. Lambert

Illinois Institute of Technology N-M-R Newsletter

No. 111
DECEMBER, 1967

OVER

Deadline Dates: No. 112: 6 January 1968
No. 113: 6 February 1968

Reminder: For the period August 10, 1967 to August 15, 1968 inclusive, all Newsletter contributions, enquiries, etc., should be addressed as follows:

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

-continued on the outside back cover

STANFORD UNIVERSITY
STANFORD, CALIFORNIA

DEPARTMENT OF CHEMISTRY

6 December 1967

POSITIONS NEEDED

It has just come to my attention that due to a "corporate readjustment", two NMR men of experience and professional competence are about to become available for employment elsewhere. Their availability is a direct, sole consequence of a department being eliminated, and in no way reflects adversely on these individual victims of the change. If anyone has positions available in the very near future, and wishes to consider these men, please telephone or write me and I will establish the connection.

Bernard L. Shapiro
Visiting Scholar
Department of Chemistry
Stanford University
Stanford, California 94305

Telephone: Office: (415) 321-2300, ext. 2512
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TELEGRAMS: VITAMINE - WEESP

N.V. **PHILIPS-DUPHAR**

POSTBUS 2 - WEESP - NEDERLAND

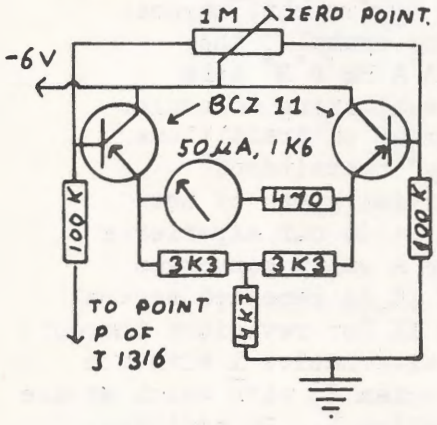
Professor B.L. Shapiro,
Department of Chemistry,
Illinois Institute of Technology,
Chicago, Illinois 60616
U.S.A.

Uw ref./Your ref. Onze ref./Our ref. FVD/AvdB/75 Afd./Dept. 56632 Datum/Date October 27, 1967

Dear Dr. Shapiro,

Continous Lock Signal Indication on a Varian HA 100

For a continous control of the lock signal the following modification is made on our Varian HA 100 equipped with autoshim. A µA-meter, in combination with an emitter follower for reducing the load, is connected with the output of the "AC amplifier and phase detector" (Point P of J 1316, schematic 87-101-737) (fig. 1). The autoshim phase detector detects the lock signal in an absorbtion mode, in contrast to the control phase detector, which detects the lock signal in a dispersion mode and whose output is held at zero by a feedback to the flux stabilizer.
By means of a resistor of 470 Ω in series with this particular µA-meter, a 1 V p-p lock signal on the scope corresponds to full scale deflection on the meter.
Plug J 1302, which has several vacant positions, is used for connecting the meter to the phase detector.



This control has the following advantages:

1) Shimming the Y and curvature gradients is effected more easily and quickly than with the shim switch on, and using the recorder; furthermore this method is much more sensitive than that of using the scope.

2) Changes in homogeneity can be observed directly during a scan.

3) A very week lock signal, hidden by noise on the scope, but sufficient for frequency sweep operation, can be detected.

Sincerely yours,

F.v. Deu

F.W. van Deursen
N.V. PHILIPS-DUPHAR
Research Laboratories,
Dept. 32.

JET PROPULSION LABORATORY *California Institute of Technology • 4800 Oak Grove Drive, Pasadena, California 91103*

November 3, 1967

Refer to: 328:SLM:ja

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Barry:

Currently there are three popular NMR programs for the IBM 7090 with 32K core which allow the iterative fitting of complex NMR spectra. These include: 1) the NMRIT and NMREN combination,[1]

1. J. D. Swalen and C. A. Reilly, J. Chem. Phys. 37, 21 (1962).

2) the equivalence factoring version of NMRIT and NMREN;[2] and

2. R. C. Ferguson and D. W. Marquardt, ibid. 41, 2087 (1964).

3) the two stage LAOCOON II method.[3] From our experience with

3. S. Castellano and A. A. Bothner-By, ibid. 41, 3863 (1964).

Programs 1 and 2 and our understanding of Program 3, it is apparent that certain inconveniences arise between stages in the analyses of spin systems containing sets of chemical shift equivalent, magnetically nonequivalent nuclei such as exist in (for example) the $AA'BB'$, $AA'BB'CC'$, $A_3A_3'BB'$, $AA'BB'B''B'''$ and $AA'A''A'''BB'B''B'''$ spin systems. In these cases, and for other cases exhibiting molecular symmetry, one must 1) consider each symmetry group of transitions separately at one stage or 2) introduce "dummy" transitions (derived from a spectrum calculated from an initial guess of the spectral parameters) between symmetry groups. It is our experience that the latter alternative may or may not give a valid converged solution for the experimental spectrum even if it is repeated several times. Not having any experience with LAOCOON II (or revisions thereof) we are not sure whether it is possible to use alternative 1 with the latter. The equivalence factoring program (Program 2) with which we are familiar is definitely not suitable for alternative 1. In addition, with Program 2 the largest cases of practical interest of the type described above which can be handled are $AA'A''BB'B''$, $AA'BB'CC'$

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and AA′A″A‴BB′. These are computed as ABCDEF cases, i.e. without symmetry. To use this program it is also necessary to introduce "dummy" transitions between symmetry groups or the resulting matrix of the equations for the energy levels is singular. Thus with spin systems exhibiting molecular symmetry it is probably best to use Program 1. For these problems, one must use NMREN-2 separately on each set of transitions belonging to a particular symmetry group. NMREN-2 must set the sum of the energy levels for each symmetry submatrix equal to zero to avoid singularity problems. Because the trace of a given symmetry submatrix is in general not zero, suitable corrections must be made manually to each submatrix to assure the complete Hamiltonian matrix is internally consistent. For large spin systems this is a lot of work.

To overcome the problems with magnetically nonequivalent nuclei described above and to generally ease the tedium of manual data transfer with NMRIT and NMREN-2, we have performed some surgery on and made some additions to the original Swalen and Reilly Program.[1] Specifically we have mated NMRIT and NMREN-2 into one master program (as yet unnamed; perhaps NMRENITPUBLISH is appropriate) which exhibits the following features:

A. It starts with one or several sets of transitions divided according to symmetry and assigned from a zero iteration NMRIT calculation. Also, it is fed a set of arbitrary trial parameters which should embody the symmetry of the spin system. It will help the convergence time if these are the best trial parameters one has in hand.

B. It calculates a set (or sets) of energy levels using NMREN-2 for each group of transitions assuming that the trace of any submatrix is equal to zero. The resultant energy levels are labeled according to symmetry group.

C. It uses the trial parameters to calculate trial energy levels. The program then computes a

$$\Delta_i^k = E_i^k\,(\text{obs}) - E_i^k\,(\text{calc})$$

where i and k are the energy level index and symmetry group index, respectively. The Δ's are then averaged:

$$\langle \Delta^k \rangle = \frac{1}{N} \sum_{i=1}^{N} \Delta_i^k$$

where N is the number of levels in symmetry group K. The $\langle \Delta^k \rangle$ are a close approximation to

$$\sum_{i=1}^{N} E_i^k$$

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and hence yield the correction factor necessary to correct for the fact that NMREN-2 assumed

$$\sum_{i=1}^{N} E_i^k = 0.$$

The program then proceeds to calculate the corrected set of observed energy levels,

$$E_i^{k\prime}\ (\text{obs}) = E_i^k\ (\text{obs}) \pm |\langle\Delta^k\rangle|$$

where the plus sign holds for negative $\langle\Delta^k\rangle$ and the minus sign for positive $\langle\Delta^k\rangle$. Using the E_i^k (obs), a new set of zero iteration Δ's are derived and the program proceeds to the iteration. A new $\langle\Delta^k\rangle$ is calculated after each iteration to adjust for errors in the relation

$$\langle\Delta^k\rangle = \sum_{i=1}^{N} E_i^k$$

D. A set of new trial parameters is derived in the usual way from the corrected experimental energy levels.

E. The whole process is repeated. Iteration is carried out until the Sum of Squares of Residuals and Average Deviation of Observed Minus Calculated Line Position have been reduced to an acceptable level or until it is obvious from large values of the above parameters that the beginning assignment was wrong.

F. This modified program cannot be used solely for a zero iteration NMRIT calculation.

G. The program has input and output formats nearly the same as the usual NMRIT.

We have tested this program on AA′BB′, AA′BB′CC′ and A_3BCD systems with extremely gratifying results. A nominal time for AA′BB′CC′ operation with ten iterations is two minutes and forty-five seconds. A detailed account of this program is being prepared. We wish to test it a little more before making it generally available. However, when preprints are available we will advertise in these letters.

One more thing before closing. We have written a routine called SORT which sorts the transitions and corresponding energy levels from a zero iteration NMRIT calculation of transitions and levels. The sorted groups will usually correspond to symmetry submatrices

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within the total Hamiltonian. The connected groups are printed out in addition to the usual NMRIT output. This will be a tremendous time saver when one begins to assemble the input data for the iterative program. In addition, it will provide a tidy table of reference for double resonance experiments. Hence, this routine should help to further reduce the "nagging backache" of routine spectral analysis.

With best regards,

Mike

Michael T. Bowers

Thelma I. Chapman

Thelma I. Chapman

Stan

Stanley L. Manatt

UNIVERSITÉ D'OTTAWA
DÉPARTEMENT DE CHIMIE

UNIVERSITY OF OTTAWA
DEPARTMENT OF CHEMISTRY

OTTAWA 2, CANADA

November 2nd, 1967

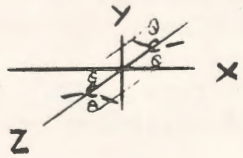
Dr. B.L. Shapiro,
Department of Chemistry,
Stanford University,
Stanford, Calif. 94305,
U. S. A.

Dear Barry:

The following is a contribution which, I hope, fulfills your requirements 2 and 3 of the classification in IITNMRN - 107-1.

Subject: The anisotropy of a C = C Bond

The current state of affairs of this topic is somewhat muddled. Bothner-By and Pople summarized the situation up to the end of 1964 in their review of diamagnetic anisotropy (1). If one labels the principal axes of susceptibility as in Fig. 1, then three different proposals regarding the effect of the double bond on neighbouring protons have been made. They are as follows:



	X	Y	Z (+ indicates shielding)
a) Jackman	-	+	-
b) Pople	-	+	+
c) Conroy	+	+	- ? (implied)

Experimental evidence in favor of shielding on the Y direction has been obtained by a number of workers. Two questions still remain undecided. Is X shielding or deshielding? Is Z shielding or deshielding? The most specific attempt to answer these questions is the work of Whalley ApSimon et al, who found (see IITNMRN - 101 for revised values) that only the Z region is deshielding, and that X and Y have approximately equal values of $\chi = -9 \times 10^{-30}$. Nevertheless there are many notable exceptions to their results, particularly in bicyclic systems. Tori and co-workers observed a non-additive effect of introducing one and two double bonds into norbornane (2) and later found that a double bond actually deshielded the proton syn to it in norbornene and benzonorbornene (3). Recently, they

cited evidence to show that there is a substituent effect on the chemical shift of the anti-proton in the 7 position of 6-substituted benzonorbornenes, which indicates the presence of a "non-classical" interaction in the ground state of this molecule (4).

It is therefore apparent that bicyclic systems do not serve as satisfactory models for the determination of principle susceptibilities, i.e. either "non-classical effects intrude, or the susceptibility of a double bond is not constant. This lack of constancy may not be restricted to the bicyclic system.

We have obtained some additional chemical shift data which reinforces the idea that the susceptibilities vary in bicyclics. The results are of course, qualitative in nature. We have not attempted any quantitative treatment of the data because of its obvious variability. The chemical shift data is given in Table 1. A summary of the correlations and anomalous effects are given in Table 2.

This work is taken from the thesis of Dr. M.Z. Haq, University of Ottawa, 1967.

Best regards,

Bob Fraser

R. R. Fraser

(1) Ann. Review of Phys. Chem., p. 54, 1964.

(2) K. Tori et al, Can. J. Chem., 42, 928 (1964).

(3) K. Tori et al, Tetr. Letters, 1966, p. 9.

(4) K. Tori et al, Can. J. Chem., 45, 1185 (1967).

(5) R.R. Fraser, Can. J. Chem., 40, 28 (1962).

TABLE I - Chemical Shifts in τ Units (10% w/v solutions in CCl_4)

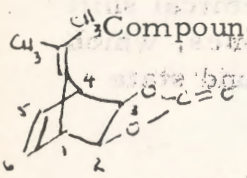
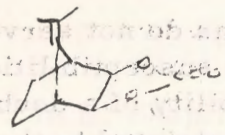
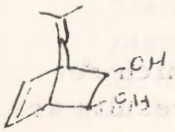
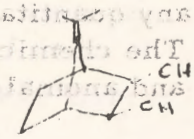
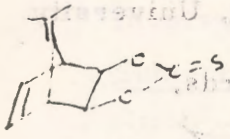
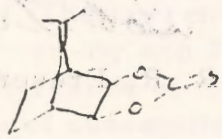
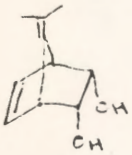
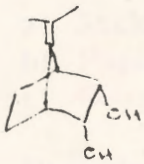
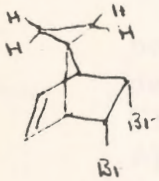
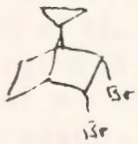
Compound	$C_{2,3}$	$C_{1,4}$	$C_{5,6}$	Methyl
I 	5.60(s)	6.50(t)	3.81(6)	8.33
II 	5.57(s)	7.20(t)	8.57(x) 8.79(n)	8.27
III 	6.34(s)	6.84(t)	3.82(t)	8.34
IV 	6.31(s)	7.43(t)	8.63(x) 8.82(n)	8.29
V 	5.18(s)	6.37(t)	3.78(t)	8.35
VI 	5.22(s)	7.05(t)	8.51(x) 8.77(n)	8.29
VII 	5.92(t)	6.51(q)	3.64(t)	8.46
VIII 	6.15(t)	7.14(q)	8.68(x) 9.12(n)	8.36
IX 	5.48(t)	7.43(q)	3.71(t)	9.46(s)
X 	5.33(m)			9.39(s)
XI 	3.26	7.08(q)		9.57(s)
XII 	3.97(t)	7.92		9.62, 9.71 (A_2B_2)
XIII 				9.58(s)

TABLE 2 - Effect of Removal of Double Bond

	$\Delta\tau_{C2,C3}$	$\Delta\tau_{cyclopropyl}$	Comment:
I → II	- 0.03		
III → IV	-.0.03		
V → VI	+ 0.04		exception to Fraser's Proposals (5)
VII → VIII	+ 0.23		
IX → X	- 0.15		Exception to Fraser's proposal
XI → XII		+ 0.05, +0.14	no additivity !
XII → XIII		- 0.04, -0.13	

THE SCHOOL OF PHARMACY

UNIVERSITY OF LONDON

PHARMACEUTICAL CHEMISTRY
PROFESSOR W. B. WHALLEY
D.Sc., Ph.D., F.R.I.C.

29/39, BRUNSWICK SQUARE
LONDON, W.C 1.
TELEPHONE TERMINUS 7651/8

JWP/vbrh

3rd November, 1967

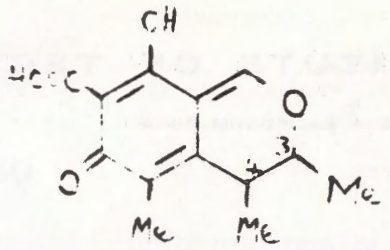
Dear Dr. Shapiro,

The Conformation of Citrinin

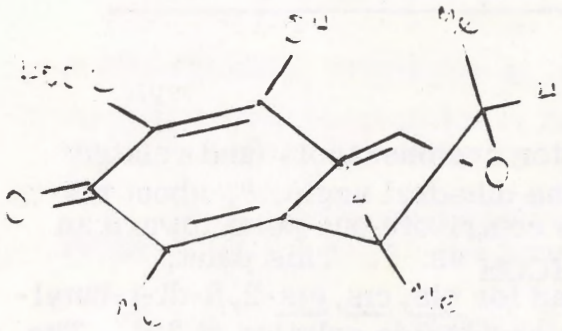
In the course of continuing work on the chemistry of citrinin (I) by members of Professor Whalley's group, we re-examined the n.m.r. on our new A60A, as a test of the decoupler set-up. As previously reported (D.W. Mathieson and W.B. Whalley, J.Chem.Soc., 1964, 4640) H-3 and H-4 appear as quartets as δ 4.82 and δ 3.03, the corresponding methyl groups appearing as doublets at δ 1.38 and δ 1.23 respectively. When either methine proton is decoupled from its neighbouring methyl group, it collapses to a sharp singlet, confirming that the coupling between H-3 and H-4 is very small (not more than ca. 1 c.p.s.).

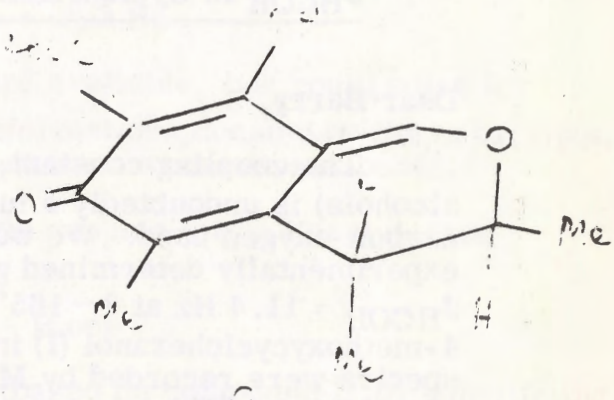
This confirms the previous conclusion that citrinin must have the two methyls in the trans relationship (the cis isomer has a dihedral angle of around 40° in both conformations), and confirms that the preferred conformation, in dueterochloroform solution, must be that depicted by A, with both methyls quasi-axial, rather than that shown at B, with quasi-equatorial methyls.

An attempt to run the spectrum of citrinin at elevated temperatures in deuterated dimethylsulphoxide was partly foiled by decomposition of the substrate. However, it is clear that the spectrum is essentially the same at 40°, 60° and 80°, showing that the energy difference between the diaxial and diequatorial conformers must be considerable. Citrinin is esentially a one conformation system up to at least 80°.



(I)





Please credit this contribution to Professor Whalley's subscription.

Yours sincerely,

J. W. Powell

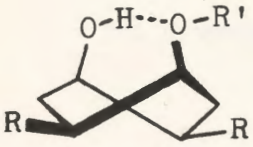
Professor B. L. Shapiro,
Department of Chemistry,
Stanford University,
Stanford, California 94305,
U.S.A.

CALIFORNIA INSTITUTE OF TECHNOLOGY

PASADENA, CALIFORNIA 91109

GATES AND CRELLIN LABORATORIES OF CHEMISTRY

October 18, 1967



	R	R'
I	t-Bu	Me
II	t-Bu	H

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

J_{HCOH} in Cyclohexanols with Transannular Hydrogen Bonds

Dear Barry,

The coupling constant, J_{HCOH}, for cyclohexanols (and related alcohols) is undoubtedly a function of the dihedral angle, θ, about the carbon-oxygen bond. We would like to contribute one point toward an experimentally determined graph of J_{HCOH} vs. θ. This point, J_{HCOH} = 11.4 Hz at $\theta \sim 165°$, was found for cis, cis, cis-2,5-di-t-butyl-4-methoxycyclohexanol (I) in carbon tetrachloride solution at 30°. The spectra were recorded by Mr. Anthony Gallo at Tufts University, by use of a Varian A-60A spectrometer with a C-1024 computer. For both I and cis, cis, cis-2,5-di-t-butyl-1,4-cyclohexanediol (II) in carbon tetrachloride solution at 30°, J_{HCOH} is independent of concentration over the wide concentration range studied:

I		II	
Concentration moles/liter	J_{HCOH} Hz	Concentration moles/liter	J_{HCOH} Hz
0.43	11.3 ± 0.2	0.086	7.0 ± 0.2
0.074	11.4 ± 0.2	0.016	6.9 ± 0.2
0.005	11.4 ± 0.3	0.005	7.0 ± 0.3
1/∞	11.4 (extrapolated)	1/∞	7.0 (extrapolated)

The infrared spectra of I and II, under similar conditions of solvent, concentration, and temperature, have been interpreted previously in terms of negligible populations of nonhydrogen bonded conformations.[1] Therefore, compound I can be considered "conformationally homogeneous", with $\theta \sim 165°$ (as measured by projection from Dreiding molecular models).

Dr. B. L. Shapiro
October 18, 1967
Page Two

However, II is not "conformationally homogeneous"; its infrared spectrum has been interpreted in terms of two pairs of equivalent intramolecularly hydrogen bonded conformations, interconverting rapidly by rotation about the carbon-oxygen bonds.[1] Therefore, for II, J_{HCOH}, 7.0 Hz, may be interpreted in terms of the average of four different environments for each hydroxyl proton, $t_1 J_{\theta_1} + t_2 J_{\theta_2} + t_3 J_{\theta_3} + t_4 J_{\theta_4} = 7.0$ Hz where t_i is the time fraction spent by a hydroxyl proton at dihedral angle θ_i, and $\Sigma t_i = 1$, $t_1 = t_3$, $t_2 = t_4$, $\theta_1 = \theta_2 \sim 165°$, $\theta_3 \sim 75°$, and $\theta_4 \sim 45°$. Setting $J_{\theta_1} = 11.4$ Hz (based on compound I), we derive:

$$t_1 J_{\theta_3} + (\tfrac{1}{2} - t_1) J_{\theta_4} = 1.3 \text{ Hz} .$$

If experimental values for J_{θ_3} and J_{θ_4} were available, one could solve for t_1, and determine populations of the four conformations, denoted by the subscripts, which are interconverting by rotation about the carbon-oxygen bonds.

As a crude approximation, one might assume that a Karplus-type relationship exists, of the form:

$$J_{HCOH} = A \cos^2\theta - B \cos\theta .$$

Then one can estimate $J_{180°} = 12.2$ Hz, (based on compound I, by substituting θ, 165°; J_{HCOH}, 11.4 Hz; $B \sim 0$). Next one can estimate $J_{60°} = 1.9$ Hz (based upon methanol in carbon tetrachloride solution,[2] for which $J_{HCOH} = 5.3$ Hz $= \frac{1}{3}[2 J_{60°} + J_{180°}]$). Then, evaluating the constants, A = 10.7, and B = 1.5; J_{HCOH} at 45°, 60°, 75°, 90°, 165°, and 180° would have values 4.3, 1.9, 0.3, 0, 11.4, and 12.2 Hz, respectively, and t_1 would be 0.21, a value in reasonable agreement with the earlier interpretation of the infrared spectra of II.[1]

This crude approximation may have heuristic value, but is not a valid substitute for experiment. Therefore, we look forward to the contribution by others of additional experimental points for the J_{HCOH} vs. θ graph in carbon tetrachloride solution at infinite dilution derived from other intramolecularly hydrogen bonded alcohols of known geometry and established conformational homogeneity.

Sincerely,

Robert Stolow

RS:hb

[1] R. D. Stolow and M. M. Bonaventura, J. Am. Chem. Soc., 85, 3636 (1963).

[2] W. B. Moniz, C. F. Poranski, and T. N. Hall, ibid., 88, 190 (1966).

Fysiska Institutionen, Uppsala, November 10, 1967

Professor Bernad L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305
USA

Spin-couplings in fluorothiophenes

Salo Gronowitz, who is now professor of organic chemistry at the University of Lund (Sweden) has for some time been interested in fluorinated thiophenes, and in collaboration with him we have studied the NMR spectra of fluorothiophenes here in Uppsala. The spectra have been investigated by use of our new HA-60-IL spectrometer.

In this letter we want to report the parameters of 2- and 3- fluorothiophene. The spin coupling constants for 2- fluorothiophene are (in Hz):

$J_{34} = 3.89$ $J_{35} = 1.69$ $J_{45} = 6.02$

$J_{2F-3} = 1.62$ $J_{2F-4} = 3.07$ $J_{2F-5} = 3.10$

and for 3- fluorothiophene (in Hz):

$J_{24} = 1.52$ $J_{25} = 3.50$ $J_{45} = 5.36$

$J_{3F-2} = 1.02$ $J_{3F-4} = -0.1$ $J_{3F-5} = 3.30$

Except for J_{3F-4} all the H-F spin coupling constants are of the same sign as the H-H spin coupling constants. The shift of the fluorine resonance of 2-fluorothiophene is 28.30 ppm and that of 3-fluorothiophene 32.05 ppm downfield from hexafluorobenzene. An isotope shift of 2- fluorothiophene due to ^{34}S was observed and is 0.014 ppm upfield. The $^{13}C-^{19}F$ spin coupling constants are 285 and 256 Hz in 2- and 3- fluorothiophene, respectively. The proton spectrum of 2- fluorothiophene is shown in Fig. 1 and the fluorine spectrum of the same compound is shown in Fig. 2.

A paper on these two monofluorothiophenes is under print in Acta.Chem. Scand. In a subsequent paper the result from an investigation of six difluorothiophenes and one trifluorothiophene will be reported.

Yours sincerely
Sören Rodmar
Sören Rodmar

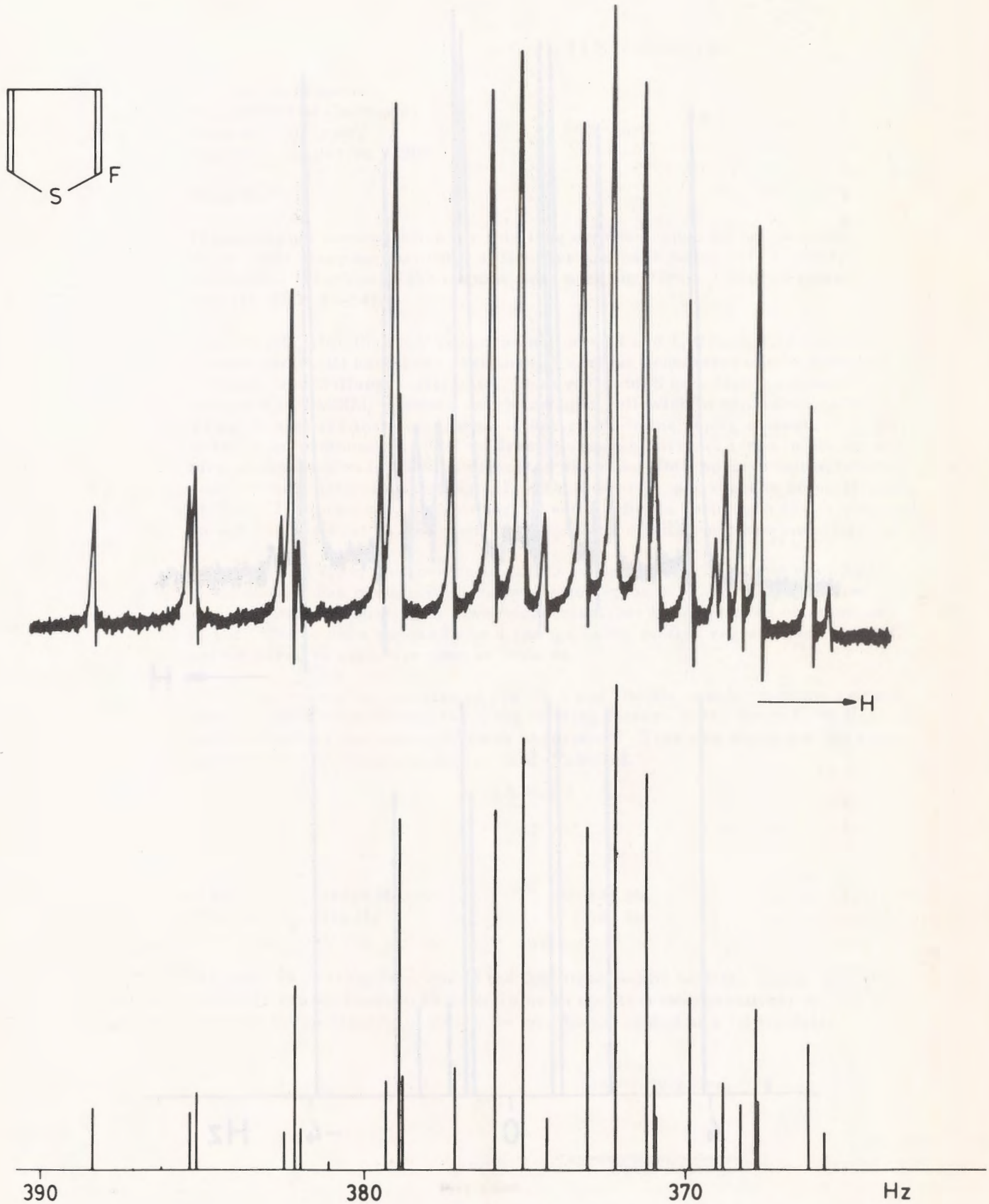


Fig. 1

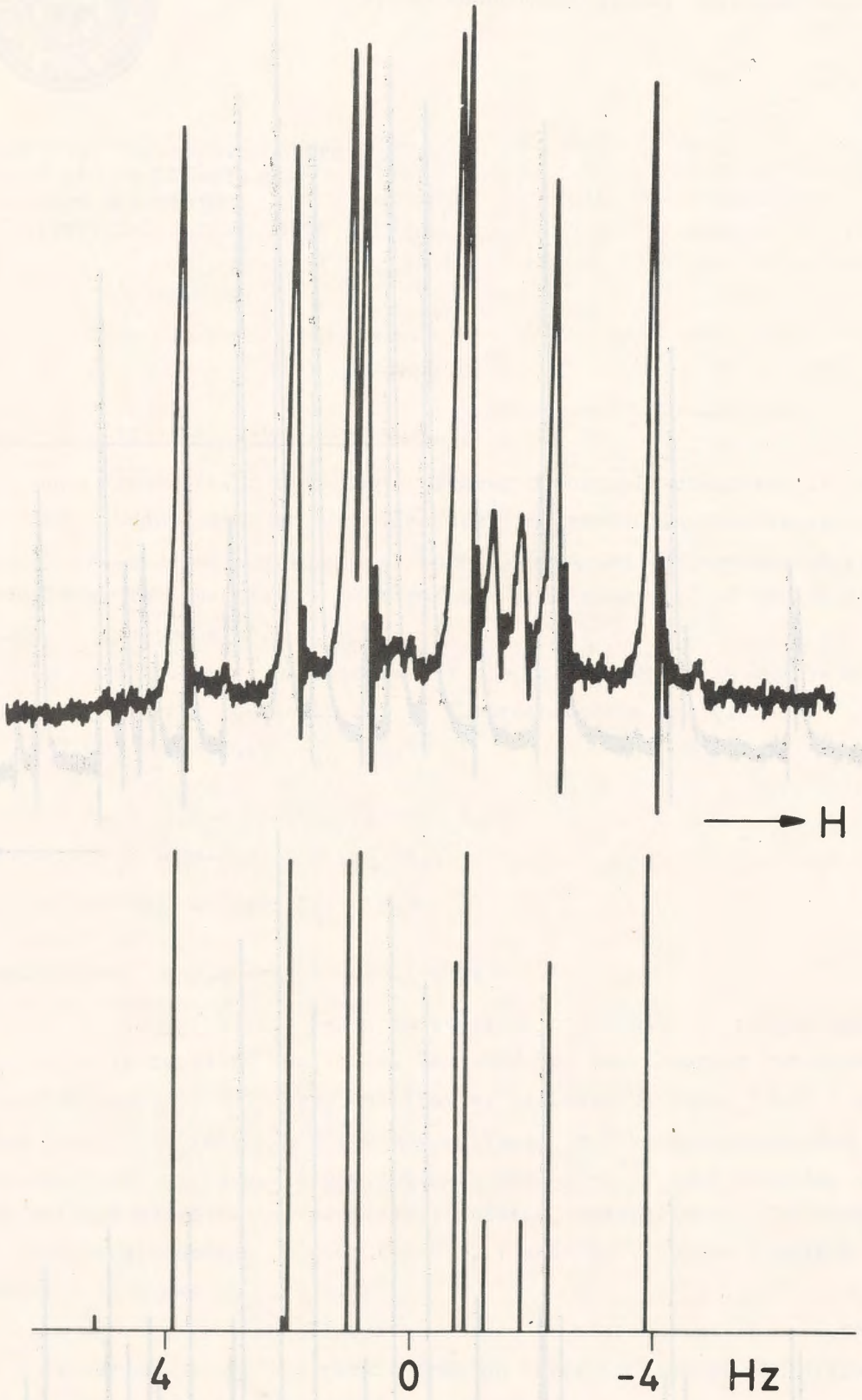


Fig. 2

FAIRCHILD
SPACE AND DEFENSE SYSTEMS
A DIVISION OF FAIRCHILD CAMERA AND INSTRUMENT CORPORATION
300 ROBBINS LANE, SYOSSET, L.I., NEW YORK 11791 · 516 WE 1-4500 · TWX 510 221-1858 · CABLE FAIRCAM SYOSSET NEW YORK

13 November 1967

Dr. B. L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Barry:

Please accept our apologies for this long overdue contribution. We have had a great many instrumental difficulties and have begun only recently to examine solutions of the cyanine dyes with our DP-IL C-1024 System (see IIT NMR 83-54).

Two dyes (1, 1'diethyl 4, 4'quinocyanine iodide I and 1, 1'diethyl, 2'quinocyanine iodide II) have been examined at various concentrations in dimethyl sulfoxide and trifluoroacetic acid. The dyes, which give highly coloured solutions in $DMSOd_6$ produce only very light yellowish brown solutions in TFA. It appears that conjugation is destroyed in the acidic solvent, possibly by protonation. That no drastic changes have occurred in dye structure on dissolution in TFA is suggested since the NMR spectra in the two solvents are quite similar (Fig. 1), with, however, some peaks being strongly shifted. Furthermore, preliminary results indicate unchanged dye is obtained on solvent evaporation. Further investigations of this point are underway.

It is apparent from the spectra in DMSO presented in Fig. 2 that very little if any change has occurred in the low-field region over the concentration range examined. Spectra at lower concentrations have not been obtained as of yet. There does appear to be a change in the methyl region which we are not prepared to comment upon at present.

Fig. 1 compares the spectra of I in TFA and DMSO. Aside from the overall shift to lower field in TFA the most striking feature is the large (+ 95 Hz) upfield shift for the bridge methine absorption. This now occurs in the same region as the methine absorption of II (Table 1),

TABLE I

	I	II
TFA	340.5 Hz	348 Hz
$DMSOd_6$	436 Hz	340 Hz

Relative shift changes occur in the low-field region with the change in solvents and will hopefully be of value in spectral interpretation. A more detailed account of this work will be presented at a future date.

Sincerely yours,

David Marr

Jim LuValle
James E. LuValle

FIG. 1

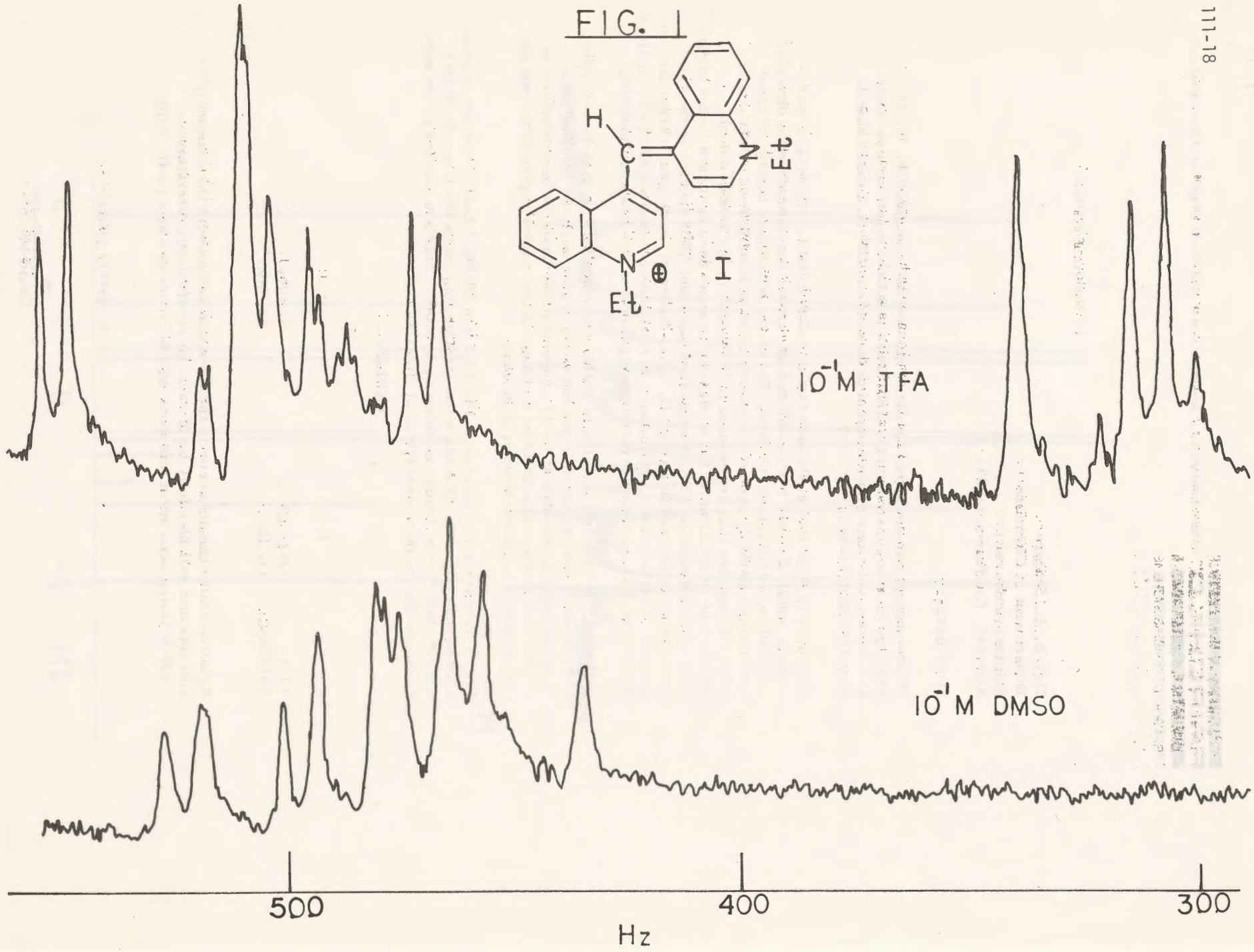
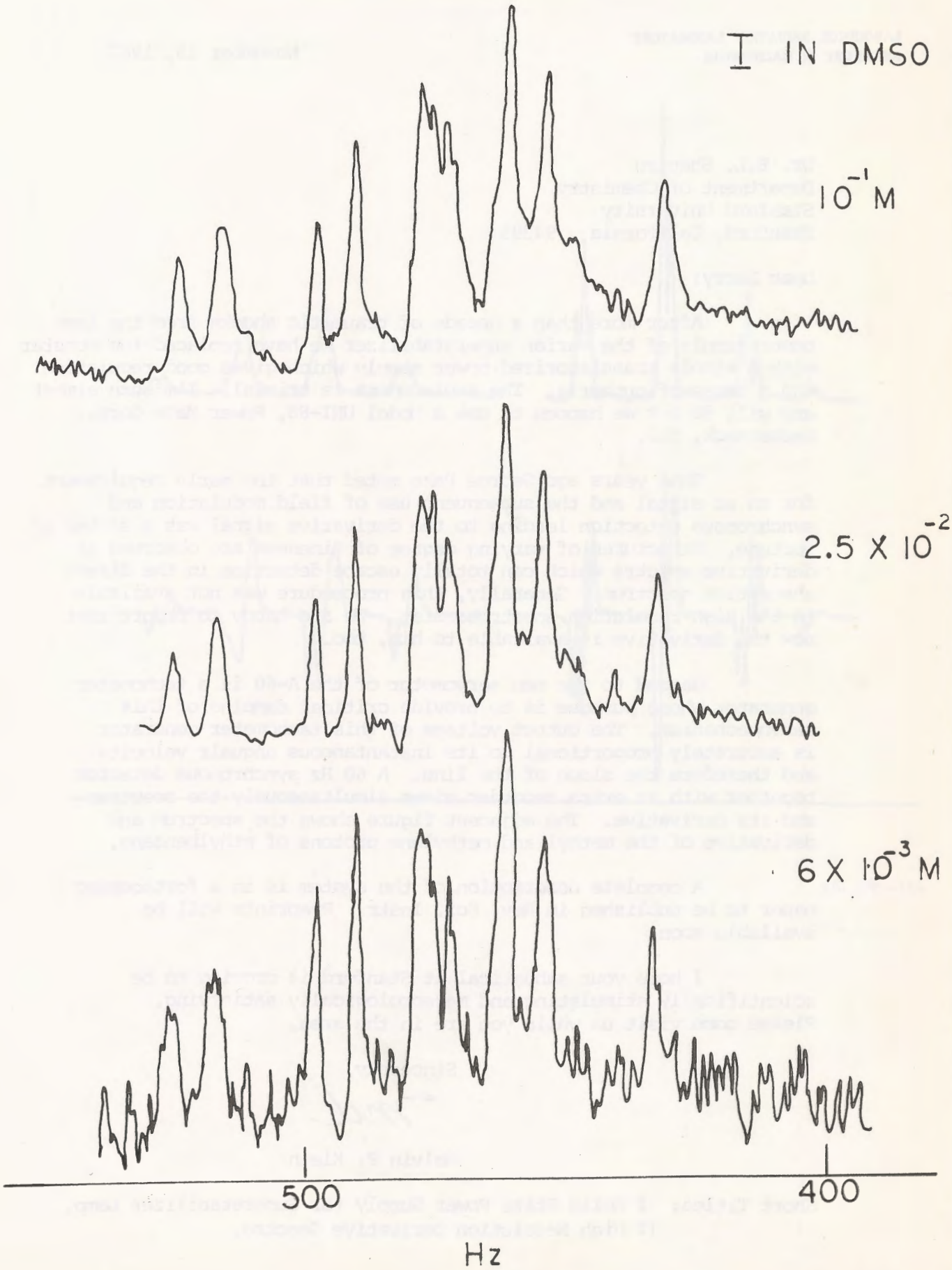


FIG. 2



UNIVERSITY OF CALIFORNIA

LAWRENCE RADIATION LABORATORY
BERKELEY 4, CALIFORNIA

November 15, 1967

Dr. B.L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94395

Dear Barry:

After more than a decade of traumatic shocks from the lamp power supply of the Varian superstabilizer we have replaced the monster with a simple transistorized power supply which gives good regulation and a sense of euphoria. The replacement is trivial. I'm sure almost any will do but we happen to use a Model UNI-88, Power Mate Corp., Hackensack, N.J.

Some years ago George Pake noted that the early requirement for an ac signal and the subsequent use of field modulation and synchronous detection leading to the derivative signal was a stroke of fortune. Structures of varying degree of fineness are observed in derivative spectra which can totally escape detection in the direct absorption spectrum. Generally, this proceedure was not available to the high resolution spectroscopist. We are happy to report that now the derivative is available to him, too.

Ganged to the pen servomotor of the A-60 is a tachometer generator whose purpose is to provide critical damping of this servomechanism. The output voltage of this tachometer generator is accurately proportional to its instantaneous angualr velocity and therefore the slope of the line. A 60 Hz synchronous detector together with an extra recorder gives simultaneously the spectrum and its derivative. The adjacent figure shows the spectrum and derivative of the methyl and methylene protons of ethylbenzene.

A complete description of the system is in a forthcoming paper to be published in Rev. Sci. Instr. Preprints will be available soon.

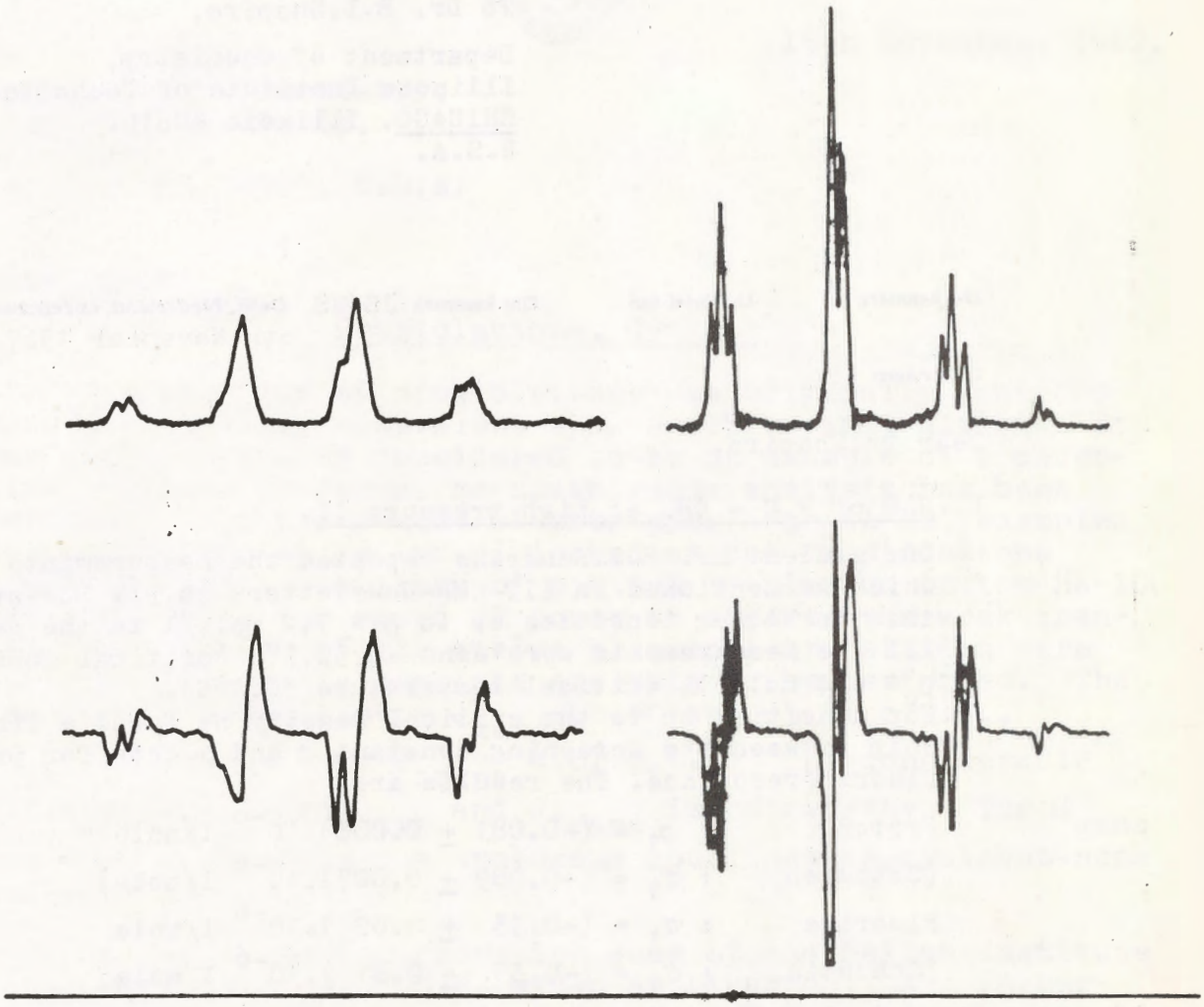
I hope your sabbatical at Stanford is proving to be scientifically stimulating and meteorologically satisfying. Please come visit us while you are in the area.

Sincerely,

Mel

Melvin P. Klein

Short Titles: I Solid State Power Supply for Superstabilizer Lamp.
II High Resolution Derivative Spectra.



XBL 676-1134

Technische Hogeschool Delft

Laboratorium voor Technische Natuurkunde

To Dr. B.L.Shapiro,

Department of Chemistry,
Illinois Institute of Technology,
CHICAGO. Illinois 60616.
U.S.A.

Uw kenmerk Uw brief van Ons kenmerk JS/WS **Delft, Nederland, Lorentzweg 1, tel. 01730-33222**
6th November 1967.

Onderwerp

Dear Dr.Shapiro,

I. NMR of $F_2C = CH_2$ at high pressure II.

Our student Mr. H.J.Hendriks repeated the measurements of Mr.Schouten, which we mentioned in IIT-NMR-Newsletters no.93. Moreover he extended them to higher densities up to ρ = 7,2 mole/l in the gasphase.
All the measurements were done at 32.5°C (critical density ρ_c = 6.4 mole/l, critical temperature 30.1°C).
For densities up to the critical density he found a linear relationship between the screening constant σ and ρ both for proton- and fluorineresonance. The results are:

Proton : $\sigma_1 = (-0.081 \pm 0.008).10^{-6}$ l/mole
(Schouten : $\sigma_1 = (-0.089 \pm 0.007).10^{-6}$ l/mole)
Fluorine : $\sigma_1 = (-0.33 \pm 0.02).10^{-6}$ l/mole
(Schouten : $\sigma_1 = (-0.35 \pm 0.01).10^{-6}$ l/mole)

At densities higher than ρ_c there seems to be a deviation from the linear behaviour of σ, possibly due to dipolar effects. We will do more experiments to check this.
The experimental value for the proton-σ_1 is in good agreement with the calculated value, about which we hope to publish soon.

II. Dielectric cavities.

Our student Mr. J.L.Harthoorn, during the last year has been buzy with devellopping cavities made from dielectric material. We expect that these cavities will be useful in experiments on e.g. the Endor-effect.
A paper concerning this matter has been submitted for publication. To those who are interested we are quite willing to send a preprint.

Drs. W.H.Wisman, Prof.Dr.J.Smidt.

THE UNIVERSITY OF LIVERPOOL
DEPARTMENT OF ORGANIC CHEMISTRY

TELEPHONE: ROYAL 6022

THE ROBERT ROBINSON LABORATORIES,
OXFORD STREET,
LIVERPOOL 7.

15th November, 1967.

Dr. B.L. Shapiro,
Department of Chemistry,
Stanford University,
Stanford,
California, 94305, U.S.A.

Dear Barry,

Propiolactone, Cyclist

The spectrum of propiolactone was originally analysed as a magnetically equivalent A_2B_2 spectrum and, although it was later generally considered to be an example of a deceptively simple spectrum, no unambiguous analysis has been performed. In the course of obtaining some AA'BB' examples during my year at Mellon, I looked at the propiolactone spectrum under conditions of maximum resolution on the HA-100 and also using increased RF power to observe the weak transitions. Eleven of the twelve allowed A transitions were observed enabling a complete analysis to be performed. The coupling constants were J_{gem} -16.40 and -5.00 c.p.s., J_{cis} 6.93 c.p.s. and J_{trans} 4.61 c.p.s. The considerable difference between J_{cis} and J_{trans} is noteworthy. The J_{gems} are very similar to the analogous couplings in cyclobutanone and oxepine.

We have been incorporating some of the Mellon Institute facilities into our N.M.R. group at Liverpool, and in particular have translated CYCLIST into KDF 9 Algol and will be happy to supply a listing and tape to anybody interested.

Yours sincerely,

R. J. Abraham

UNION CARBIDE

UNION CARBIDE CORPORATION

P. O. BOX 278, TARRYTOWN, N. Y. 10591

UNION CARBIDE
RESEARCH INSTITUTE

November 17, 1967

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Barry:

These days I hesitate to write about anything so dated as pencil and paper analysis of high-resolution NMR spectra, although from it one can often gain insight into a problem that computers merely solve. The ABK_n system can serve both to illustrate my point and tidy up a bit of history. To do this we consider how the systematic analysis of an ABX_n system is affected by second-order terms, obtained by generalizing the ABK problem treated by Reilly and Swalen[1].

---

[1] C. A. Reilly and J. D. Swalen, J. Chem. Phys. 32, 1378 (1960)

The first-order spectrum is summarized in Table I; one can generally proceed here by picking out n + 1 AB subspectra corresponding to each fixed eigenvalue M of the X-group spin; the outer members of each subspectrum are split by J_{AB}, alternate numbers are separated by the parameter $2C_M$ defined in Table I, and the centers of successive subspectra are displaced by $1/2\,|J_{AX} + J_{BX}|$. This information plus the shifts $\nu_o\delta_X$ and $1/2\,\nu_o(\delta_A + \delta_B)$ is sufficient to complete the analysis, including the relative signs of J_{AX} and J_{BX}. The second order corrections to the energies of the four AB levels associated with a fixed quantization (F,M) of the X_n group spins are summarized below:

State	Energy Correction
(F,M,1)	$1/4[F(F+1) - M(M+1)](a^2 + b^2)$
(F,M,0)	$1/4(a^2 - b^2)\cos 2\theta_M[F(F+1) - M^2] - 1/2\,Mab\sin 2\theta_M - 1/4M\,(a^2 + b^2)$
(F,M,0')	$-1/4(a^2 - b^2)\cos 2\theta_M[F(F+1) - M^2] + 1/2\,Mab\sin 2\theta_M - 1/4M\,(a^2 + b^2)$
(F,M,-1)	$-1/4[F(F+1) - M(M-1)]\,(a^2 + b^2)$

$$a^2 = J_{AX}^{\ 2}\ \Delta^{-1} \qquad b^2 = J_{BX}^{\ 2}\ \Delta^{-1} \qquad ab = J_{AX}J_{BX}\ \Delta^{-1}$$

$$\Delta = \nu_o[1/2(\delta_A + \delta_B) - \delta_X]$$

From these we correct the four frequencies in any (AB) subspectrum by:

$$\Delta\nu(0 \longrightarrow 1) = 1/2\ [F(F+1) - M^2](a^2 \sin^2\theta_M + b^2\cos^2\theta_M) + Mab \sin 2\theta_M = \Delta\nu(-1 \longrightarrow 0')$$

$$\Delta\nu(0' \longrightarrow 1) = 1/2\ [F(F+1) - M^2](a^2\cos^2\theta_M + b^2 \sin^2\theta_M) + Mab \sin 2\theta_M = \Delta\nu(-1 \longrightarrow 0)$$

The values of J_{AB} obtained from the outer splittings are thus unaffected by second order corrections. The parameter C_M are corrected by:

$$Mab \sin 2\theta_M - 1/2\ [F(F+1) - M^2](a^2 - b^2) \cos 2\theta$$

Other second order shifts and splittings are easily calculated.

An often encountered example is the ABX_3 spectrum of ethyl groups in which the methylene protons are non-equivalent due to different rotational averaging over an assymmetric environment.[2] Here the first-order analysis shows that $J_{AX} \simeq J_{BX}$, so that

---

(2) F. Kaplan and J. D. Roberts, J. Am. Chem. Soc. 83, 4666 (1961)

---

the second-order correction to $2C_M$ is very nearly equal to $Mab \sin 2\theta_M = Mab\ J_{AB}/2C_M$, which, since J_{AX} and J_{BX} are of the same sign, has the sign of M and J_{AB}. Differences in first-order values for successive C_M are accordingly increased or reduced depending on the sign of J_{AB}. Since these differences must vanish if $J_{AX} - J_{BX} = 0$, the condition that $J_{AX} = J_{BX}$ in these systems specifies the sign of the second-order correction and hence that of J_{AB}. In retrospect, we can therefore see the conditions that led to this first clear demonstration that geminal and vicinal proton couplings were of opposite sign.

Sincerely yours,

E. B. Whipple

EBW/sr

P.S. A suitable title (ignoring the contradiction in terms) would be "Second-order ABX_n Spectra".

TABLE I

FIRST-ORDER ABX_M SPECTRA

Transition	Frequency	Intensity
${}^{1}(S)_M - {}^{0}(S)_M$	$1/2\nu_o(\delta_A+\delta_B) + 1/2J_{AB} + 1/2M(J_{AX}+J_{BX}) \mp C_M$	$\xi_M\ (1 \pm \sin 2\theta_M)$
${}^{0}(S)_M - {}^{-1}(S)_M$	$1/2\nu_o(\delta_A+\delta_B) - 1/2J_{AB} + 1/2M(J_{AX}+J_{BX}) \pm C_M$	$\xi_M\ (1 \pm \sin 2\theta_M)$
${}^{1}(S)_{M+1} - {}^{1}(S)_M$	$\nu_o\delta_X + 1/2(J_{AX} + J_{BX})$	$2^{N-1}N$
${}^{-1}(S)_{M+1} - {}^{-1}(S)_M$	$\nu_o\delta_X - 1/2(J_{AX} + J_{BX})$	$2^{N-1}N$
${}^{0}(S)_{M+1} - {}^{0}(S)_M$	$\nu_o\delta_X \pm (C_{M+1} - C_M)$	$\xi_M(1/2N+M)\cos^2(\theta_{M+1}-\theta_M)$
	$\nu_o\delta_X \pm (C_{M+1} + C_M)$	$\xi_M(1/2N+M)\sin^2(\theta_{M+1}-\theta_M)$

$$(2C_M)^2 = [\nu_o(\delta_A-\delta_B) + M(J_{AX}-J_{BX})]^2 + J_{AB}^{\ 2}$$

$$2C_M \sin 2\theta_M = J_{AB}$$

$$\xi_M = \frac{N!}{(1/2N + M)\,!\,(1/2N - M)\,!}$$

DUQUESNE UNIVERSITY
PITTSBURGH, PENNSYLVANIA
15219

November 17, 1967

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Barry: Exchange Kinetics of N-acetylglycine N-methyl amide

Thanks for the reminder note about the IIT NMR Newsletter. I was in the Far East this summer, and time seems to pass ever so quickly.

Recently Dr. James E. Bundschuh (now at the University of Illinois in Chicago) carried out studies evaluating the proton exchange kinetics of the amino protons of N-acetylglycine N-methylamide (AGMA) in aqueous solution in the pH range 0.05 to 1.70, at our laboratory. The mean life-time, T, of a proton on a particular site can be determined by observing how much it disturbs the NMR signal of an adjacent site. AGMA has two amino protons in separate environments labeled in the following manner

$$CH_3CONH\underset{(A)}{CH_2}CONH\underset{(B)}{CH_3}$$

The collapse of the doublet of the methylene protons adjacent to site A and the collapse of the doublet of the methyl adjacent to site B were taken as measures of the mean life-times for the corresponding N-H. The measured quantities were the peak width at half-height and the peak separation of a doublet. Each of the components of the N-methyl doublet actually consists of a closely spaced triplet with spin-spin interaction of 0.45 cps between the methylene and N-methyl hydrogens. Nevertheless equations for the exchange broadening of a doublet were used, and the triplet splitting was taken into account by the introduction of an effective natural line-width of the magnitude of the width of the multiplet. Fine splitting was not observed for the $N-CH_2$ doublet, possibly because of coupling from two directions, i.e., $N-CH_3$ and $C-CH_3$.

Plots of log 1/T vs. -log (HCl) show that there is a 1.3-1.4 power dependence of the specific rate on hydrogen ion concentration for both sites A and B of AGMA. The exchange reactions may be written

$$CH_3CONHCH_2CONHCH_3 + H_3O^+ = CH_3CONHCH_2CON^+H_2CH_3 + H_2O$$

$$CH_3CONHCH_2CONHCH_3 + 2H_3O^+ = CH_3CON^+{}_AH_2CH_2CON^+{}_BH_2CH_3 + 2H_2O$$

The activation energies for sites A and B are calculated to be 16.2 and 17.7 kcal/mole, respectively.

Sincerely yours,

Norman

Norman C. Li
Professor of Chemistry

NCL/fl

UNIVERSITÉ DE LYON - FACULTÉ DES SCIENCES

PHYSIQUE GÉNÉRALE

18, QUAI CLAUDE-BERNARD, 18
LYON - (7e)

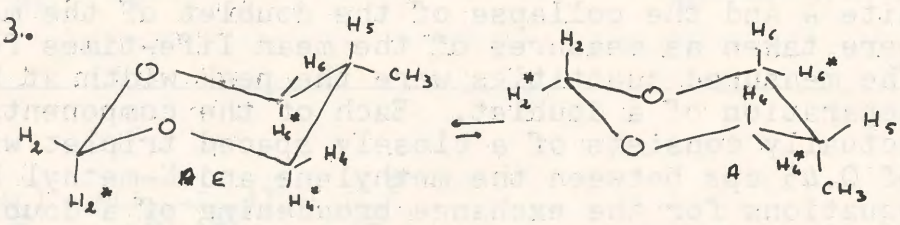
TÉLÉPHONE (LYON 78) 72-05-48

Docteur Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Ref.: Différence d'énergie libre entre méthyles axiaux et équatoriaux dans des hétérocycles.

Cher Monsieur,

Il nous semble que certains lecteurs pourraient être interessés par la différence d'énergie libre entre méthyles axiaux et équatoriaux en position 5 dans des dioxannes 1,3. Pour cette détermination nous avons étudié l'équilibre des 2 conformères du méthyl5_dioxanne_1,3.



A température ordinaire l'équilibre apparait fortement déplacé en faveur de la forme E ; cela se voit sur les couplages vicinaux et à distances ainsi que sur les déplacements chimiques.
Le dosage peut s'effectuer en regardant J_{5-6^*} comme une moyenne des constantes J_{aa} de la forme E et J_{ee} de la forme A. La constante J_{ee} a été extraite de produits similaires et prise égale à 1,5 cps , tandis que la constante J_{aa} a pu être déterminée directement sur la forme E à - 100°C : J_{aa} = 11,3 cps.

Ces valeurs conduisent à 80% de forme E à la température ordinaire soit à $\Delta G^\circ = 0,83$ kcal/mole . Cette valeur est pratiquement identique à celle observée par Eliel et ses collaborateurs (1)(: $\Delta G^\circ = 0,84$ kcal/mole) au moyen d'équilibration d'isomères du tertiobutyl-2- méthyl-5- dioxanne. Un dosage sur les méthyles confirme bien cette valeur de ΔG° : A - 100° C on observe environ 5% de forme A .

Amitiés,

J. DELMAU.

(1) E. L. ELIEL and S. M. C. KNOEBER J.Am. Chem. Soc. 88 5345 1966

Abteilung für Molekülspektroskopie
am Institut für Organische Chemie
der Technischen Hochschule Braunschweig
Abteilungsvorsteher:
apl. Prof. Dr. H.-H. Perkampus

33 Braunschweig
Schleinitzstraße
Telefon (05 31) 4 78 28 84

15. November 1967

Sehr geehrter Herr Professor Shapiro!

Im Zusammenhang mit unseren Untersuchungen über die zwischenmolekulare Wechselwirkung von Alkoholen mit heterocyclischen π-Elektronensystemen haben wir die Verschiebung der Protonensignale des Methanols bei der Verdünnung mit mehreren heterocyclischen Ringsystemen untersucht. Die Ergebnisse dieser Verdünnungsreihe sind gegen den Molenbruch des Verdünnungsmittels in Abbildung 1 und 2 dargestellt. Die Lage des OH-Signals verschiebt sich infolge des Aufbrechens der Wasserstoffbrücken sehr stark zu höherem Feld (Kurve II in Abb. 1). Bei Verdünnung mit Benzol wird dieser Effekt durch die zusätzliche diamagnetische Abschirmung des Aromaten verstärkt. Thiophen verhält sich ganz analog. Starke Abweichungen gegenüber diesen Lösungsmitteln zeigen die Stickstoffheterocyclen. Pyridin gibt im Gegensatz zum Benzol eine Verschiebung des OH-Protonensignals zu niederen Feldern, während Pyrrolderivate eine zusätzliche Verschiebung zu höherem Feld zeigen. Weniger stark, aber in gleicher Richtung werden die Protonen der Methylgruppe verschoben (Abb. 2). Dieses unterschiedliche Verhalten läßt sich durch die Annahme deuten, daß bei Pyridin die Assoziation mit Methanol in der Molekülebene erfolgt und bei den Pyrrolderivaten das Methanol von oben am Molekül angelagert wird. Der Grund für diese unterschiedliche Assoziation dürfte dadurch gegeben sein, daß einmal das für die Assoziation befähigte Elektronenpaar nach außen liegt (Pyridin) und im anderen Fall durch Einbeziehung in das π-Elektronensystem im Ringinnern liegt (Pyrrolderivate).

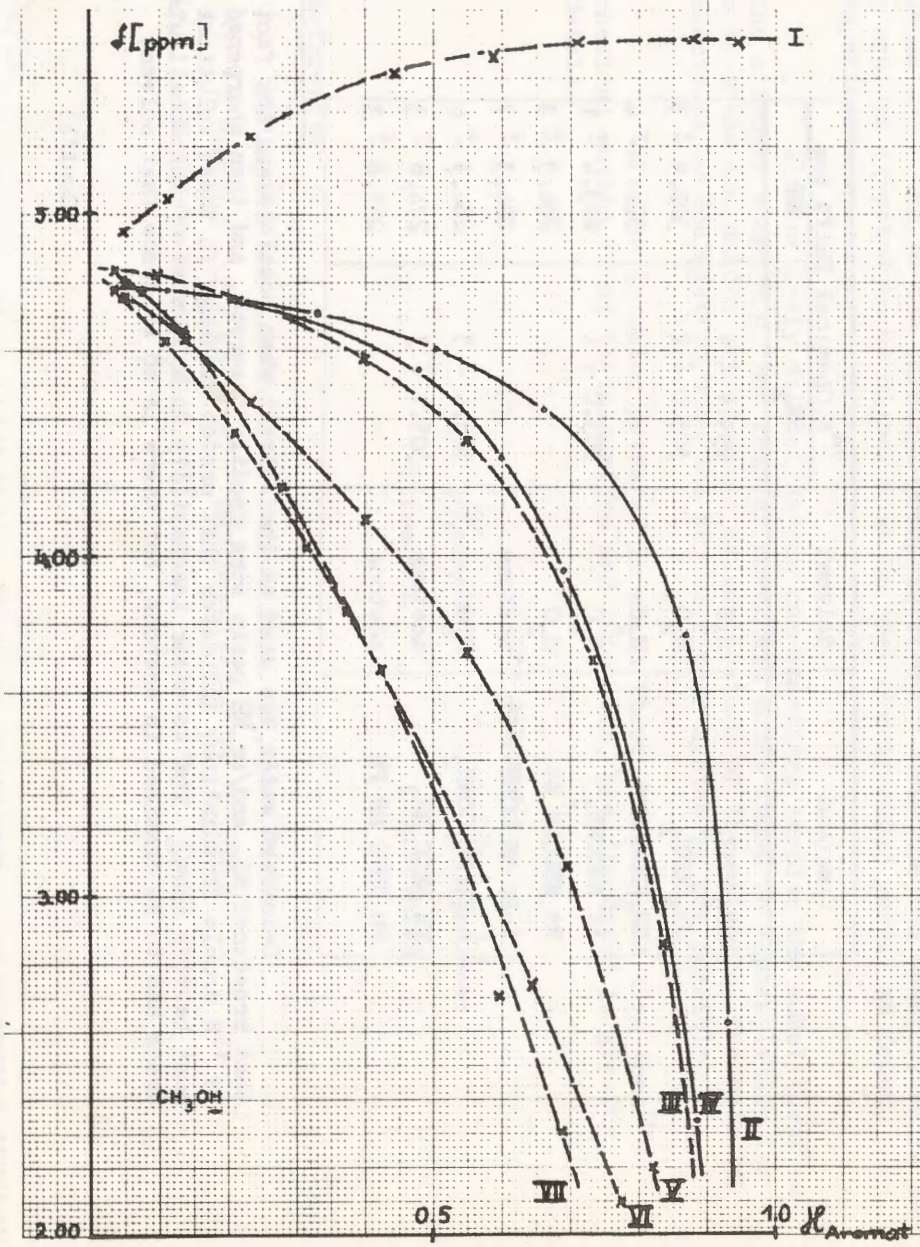
Mit freundlichen Grüßen

H.-H. Perkampus

(Prof. Dr. H.-H. Perkampus)

Uwe Krüger

(Dr. U. Krüger)



METHANOL IN

I PYRIDIN

II CCl_4

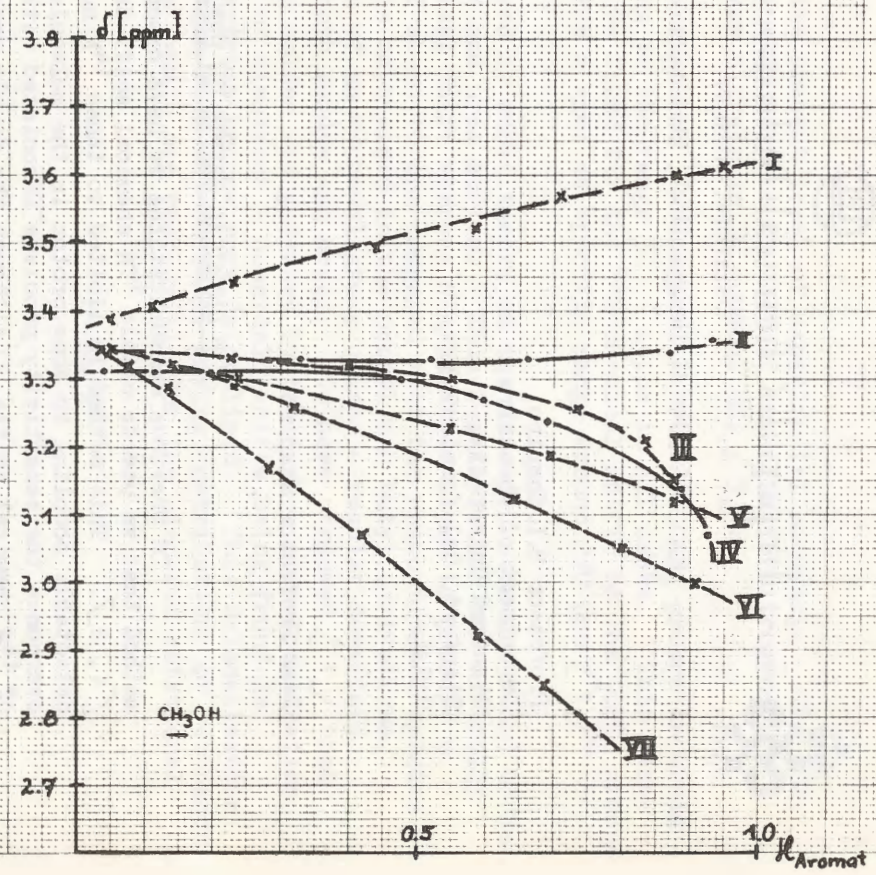
III THIOPHEN

IV BENZOL

V N-METHYLPYRROL

VI PYRROL

VII INDOL



Imperial Chemical Industries Limited
DYESTUFFS DIVISION
P.O. Box 42, Hexagon House, Blackley, Manchester, 9

Professor B.L.Shapiro,
Department of Chemistry,
Stanford University,
Stanford, California 94305,
U.S.A.

Your Ref:

Our Ref: ARG/B5
Research Department.

21st November, 1967

Dear Professor Shapiro,

^{14}N CHEMICAL SHIFTS IN UREAS

In previous communications we have described the double resonance method that we use to obtain ^{14}N chemical shift data from proton spectra [1, 2]. This method is limited to those ^{14}N nuclei which show a detectable coupling to some proton in the molecule, but it very largely overcomes the sensitivity problems associated with the direct observation of ^{14}N chemical shifts. Although the double resonance method can fail when the nitrogen quadrupole relaxation rate, or the proton exchange rate if a labile proton is involved, is too fast, we have found that it can still be used to advantage for many classes of compound. The ^{14}N chemical shifts of some ureas are shown in the Table.

Compound	Solvent	^{14}N Chemical Shift ppm	
		NH_2	NH
NH_2CONH_2	H_2O	299.1 ± 1	
CH_3CONH_2	H_2O	303.0 ± 2	302.9 ± 3
$CH_3NHCONHCH_3$	H_2O		304.7 ± 4
Et $NHCONH_2$	H_2O	303.0 ± 1	283.4 ± 1
Et NHCONH Et	H_2O		284.3 ± 3
i-Pr NH CONH-i-Pr	acetone		284.3 ± 7
n-Bu NH $CONH_2$	H_2O	306.4 ± 3	284.3 ± 4
Ph NHCO NH_2	acetone	305.1 ± 3	274.6 ± 3
Ph NHCO NH Ph	acetone		269.8 ± 3

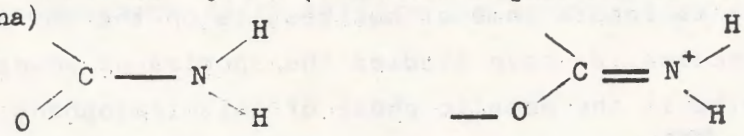
Deionised water was used as the solvent when possible and the fact that broadened NH_2 and/or NH peaks were readily observed, and then sharpened by ^{14}N double irradiation, indicates that proton exchange in these solutions must be very slow. Due to their insolubility in H_2O, some of the substituted ureas had to be examined in acetone, but there is no evidence that solvent

(Cont'd)

effects are important at the present level of experimental accuracy. The ^{14}N chemical shifts are quoted with respect to that of the nitrate nitrogen of a 4.5M solution of AR ammonium nitrate in 3N aqueous HCl [3].

The results show that the ^{14}N chemical shifts of $CONH_2$ groups in ureas are quite specific, falling in the range 303 ± 4 ppm in all cases. This range is higher than that which we found for the ^{14}N chemical shifts of the $CONH_2$ groups in primary amides which have a similar specific range around 270 ppm [1].

The changes caused by substituents on the nitrogen atom are found to be parallel in both the amide and urea series. Thus N-methylation has virtually no effect on the ^{14}N chemical shift whereas N-ethylation seems to produce a regular downfield shift of about 16 ppm compared with the unsubstituted species and this downfield shift is maintained in the propyl and butyl derivatives. Similarly the introduction of an N-phenyl group causes a regular downfield shift of about 30 ppm in both amides and ureas. We have proposed [1] that ^{14}N chemical shifts in the amides are governed by the degree of delocalisation of the nitrogen lone pair of electrons - downfield shifts being found in situations where these electrons become more delocalised. This delocalisation can take place by conjugation with the carbonyl giving contributions of resonance structure II to the system (which are responsible for the hindered rotational phenomena)



I II

In the ureas the delocalisation of any nitrogen lone pair of electrons by forms such as II will be less than in amides since two competing nitrogen atoms are bound to the carbonyl group involved. Thus the ^{14}N chemical shift in a urea is expected to be higher than in the corresponding amide, as found experimentally.

Alternatively delocalisation can sometimes involve the substituent on the nitrogen atom, e.g. the regular downfield shift found on N-phenylation for both ureas and amides arises since delocalisation of the nitrogen lone pair of electrons by conjugation with the π - electron system is now possible.

A paper is being prepared in which these effects, and also the ^{14}N chemical shifts found in thioamides and thioureas, are discussed in greater detail.

Yours sincerely,

P. Hampson A. Mathias

P.Hampson A.Mathias

References

(1) P.Hampson and A.Mathias. Molec. Phys. II, 541, 1966.

(2) P.Hampson and A.Mathias. NMR Newsletter 25, 1, 1966.

(3) D.Herbison-Evans and R.E.Richards. Molec. Phys. 8, 19, 1964.

AM./LA.

PHYSIKALISCHES INSTITUT
DER UNIVERSITÄT BASEL
KLINGELBERGSTRASSE 82 — TEL. 430422
VORSTEHER: PROF. DR. P. HUBER

Prof. Dr. P. Diehl

Dr. C.L. Khetrapal

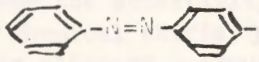
Basel, November 22, 1967

Prof. Bernard L. Shapiro
Department of Chemistry
Stanford University

Stanford Calif. 94305

Re: Spectra of Oriented Molecules - Temperature, Concentration and spinning speed dependence

Dear Barry,

We would like to report some of our results on the NMR spectra of oriented molecules. We have studied the spectra of several molecules oriented in the nematic phase of anisoleazophenyl-n-capranat (CH_3O-  -N=N--O - C(=O) - C_5H_{11}) and find the following:

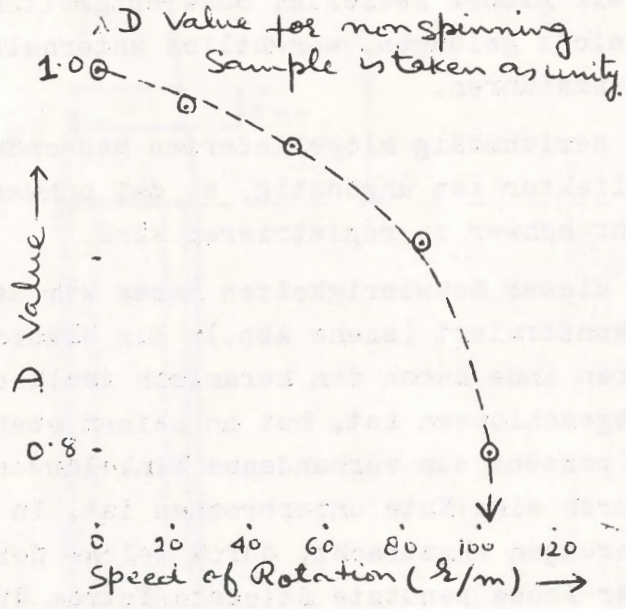
1. The spectra can be recorded from about 50° C to 90° C for a 10 mole % solution. For all the compounds studied (liquids or solids) the relative change of the degree of orientation as a function of temperature lies on approximately the same straight line (decreasing with the increase of temperature). It therefore appears that this change is a characteristic property of the liquid crystal solvent and not the solutes.

2. We notice a large concentration dependence of the degree of orientation in this liquid crystal. The orientation decreases as the concentration increases and the change may be over 30 % in some cases.

It is therefore evident that for all the work on oriented molecules, it is <u>essential</u> to mention the <u>concentration</u> along with the temperature. The large temperature and concentration dependence on the other hand could be used for the analysis of the spectra of oriented molecules since it allows the distinction between the temperature and concentration dependent D values and the normally temperature and concentration independent J

values. The concentration dependence is also important for internal references since even a slight addition of tetramethyl silane causes a change in orientation.

3. As pointed out by Burnell and de Lange in IIT NMR Newsletter No.109 the spectra can be obtained by spinning the samples. We found that the rate of spinning should not exceed 120 revolutions per minute (r/m). It may be pointed out that not only the speed of rotation should be kept constant while recording the spectra but it should be precisely known and indicated in publication since the degree of orientation varies drastically with the speed of rotation. A plot of D value versus the rate of rotation for a typical solution of a compound at a particular temperature is given below:



Yours sincerely,

Peter

(P. Diehl)

C.L. Khetrapal

(C.L. Khetrapal)

Institut für Physikalische Chemie
der Rhein.-Westf. Techn. Hochschule Aachen
Direktor Prof. Dr. U. Franck
Dozent Dr. R. Kosfeld

51 Aachen, den 27. 11. 1967
Templergraben · Fernruf (0241) 422/2150
Fernschreiber: 0832/704

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
S t a n f o r d
California 94305

Tieftemperaturmessung mit dem DA 60

Sehr geehrter Herr Dr. Shapiro,
haben Sie recht herzlichen Dank für Ihren Brief vom 10. 10. 1967.

Bei NMR-Messungen in Festkörpern im Bereich tiefer Temperaturen haben wir bisher zweierlei Schwierigkeiten gehabt:

a) Es ist uns nicht gelungen, wesentlich unterhalb - 60 °C Messungen auszuführen.

b) Der bei den serienmäßig mitgelieferten Meßsonden vorhandene Füllfaktor ist ungünstig, so daß schwache Signale nur sehr schwer zu registrieren sind.

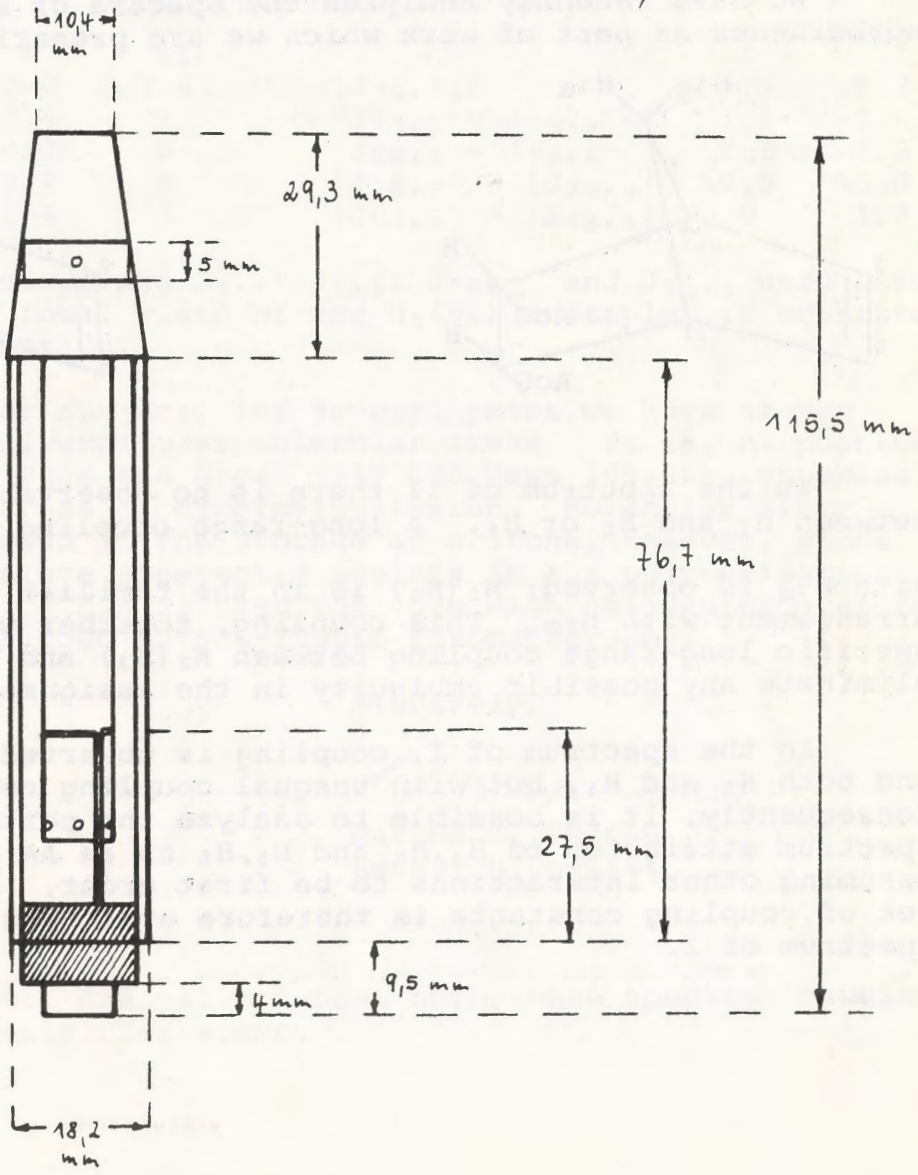
Zur Vermeidung dieser Schwierigkeiten haben wir den folgenden Insert konstruiert (siehe Abb.): Ein Glasrohr, das an seinem unteren Ende durch den keramisch isolierten Steckkontakt abgeschlossen ist, hat an seinem oberen Ende einen Schliff (passend zum vorhandenen Winkeldewar), der in der Mitte durch eine Nute unterbrochen ist. In dieser Nute sind 4 Bohrungen angebracht, durch welche der zur Temperierung der Probe benutzte Stickstoffstrom über ein Winkeldewar in den Probenraum einströmen kann. Der Kühlstrom, der zwischen Außenrohr und Innenrohr an der Meßspule vorbeiströmt, gelangt über 4 Bohrungen, die sich etwa 10 - 12 mm unterhalb der Meßspule (2 Wdg. bei 60 MHz) befinden, in den eigentlichen Probenraum; strömt an der

Probe vorbei und tritt oben aus dem Meßkopf aus. Mit dieser Temperiermeßsonde gelingt es leicht, kontinuierlich zwischen - 160 °C und + 160 °C Breitlinien-Spektren von ^{1}H und ^{19}F enthaltenden Festkörpern zu registrieren.

Auf einen unbedeutenden Nachteil, der aber durch den besseren Füllfaktor und die kontinuierliche Temperaturregelung mehr als wett gemacht wird, muß noch hingewiesen werden. Die Leakage muß nach jeder Temperaturänderung nachjustiert werden.

Abschließend will ich noch vermerken, daß das 5. Kolloquium über Kernresonanz-Spektroskopie vom 8. - 11. April 1968 in Aachen stattfinden wird.

Mit den besten Grüßen
Ihr



Southern Research Institute

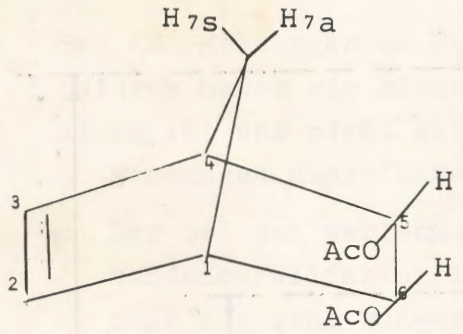
2000 NINTH AVENUE SOUTH
BIRMINGHAM, ALABAMA 35205
TELEPHONE 205-323-6592

November 28, 1967

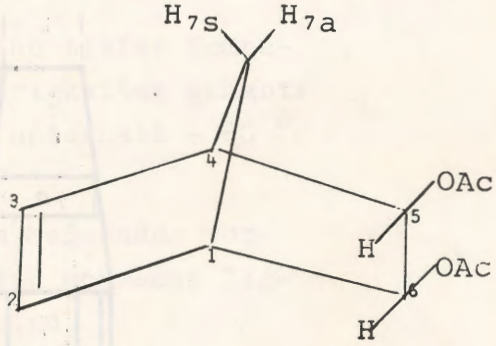
Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Barry:

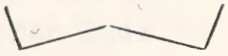
We have recently analyzed the spectra of some substituted norbornenes as part of work which we are preparing for publication.



I



II

In the spectrum of II there is no observable coupling between H_1 and H_5 or H_6. A long-range coupling of $H_5(H_6)$ with H_{7s} is observed; $H_5(H_6)$ is in the familiar  arrangement with H_{7s}. This coupling, together with the stereospecific long-range coupling between $H_2(H_3)$ and H_{7a}, appear to eliminate any possible ambiguity in the assignment of H_{7s} and H_{7a}.

In the spectrum of I, coupling is observed between $H_1(H_4)$ and both H_5 and H_6, but with unequal coupling constants. Consequently, it is possible to analyze the portion of the spectrum attributed to H_1,H_4 and H_5,H_6 as an AA'XX' spectrum assuming other interactions to be first order. A more complete set of coupling constants is therefore available from the spectrum of I.

Dr. Bernard L. Shapiro
Stanford, California 94305
November 28, 1967

Southern Research Institute

In addition, our analyses of these spectra confirm the conclusion of Dr. Marchand with reference to the relative chemical shifts of H_{7a} and H_{7s} (IIT NMR News 107-39), since we find that H_{7s} is downfield from H_{7a} in I, but upfield from H_{7a} in II. This is particularly interesting since the conformations of our compound are analogous to those of Dr. Marchand.

Chemical Shifts (ppm downfield from TMS)

Compound	H_1, H_4	H_2, H_3	H_5, H_6	H_{7a}	H_{7s}
I	3.12	6.20	5.22	1.36	1.58
II	2.82	6.16	4.73	2.03	1.72

Coupling Constants (Hz)

	I	II		I	II
$\lvert J_{1,2} + J_{1,3} \rvert$	3.8	3.4	$\lvert J_{7a,7s} \rvert$	9.9	9.2
$J_{5,6}$	7.4	-	$J_{7a,1} = J_{7a,4}$	1.5	1.6
$J_{1,6} = J_{4,5}$	4.0	0	$J_{7s,1} = J_{7s,4}$	2.1	1.5
$J_{1,5} = J_{4,6}$	-0.2	0	$\lvert J_{7a,2} \rvert = \lvert J_{7a,3} \rvert$	∿0.5	∿0.6
$J_{1,4}$	1.4	0	$\lvert J_{7s,5} \rvert = \lvert J_{7s,6} \rvert$	0	1.8

Vicinal couplings $J_{5,6}$; $J_{1,6}$; $J_{7s,1}$ and $J_{7a,1}$ were assumed positive. The total width of the $H_1(H_4)$ multiplet is consistent with this assumption.

On another subject, for several years we have stored most of our solvents over molecular sieve. It is, as pointed out by Doctors Page and Green (IIT NMR News 109-36), especially helpful in the case of dimethylsulfoxide. Molecular sieve should not be used in the storage of acetone, however, since the molecular sieve apparently assists in the polymerization of the acetone. This is also the case with hexadeuteroacetone, as we have confirmed by gas-liquid chromatography.

Sincerely,

Martha C. Thorpe
Research Chemist

MCT/ss

Suggested title: Analysis of some norbornene spectra; caution in the use of molecular sieve.

111-40 RRD/JKS

Ministry of Technology
NATIONAL PHYSICAL LABORATORY
TEDDINGTON, Middlesex
Telex: 262344 Telegrams: Bushylab, Teddington, Telex
Telephone: TEDdington Lock 3222, ext. 907

OUR REF:
YOUR REF:

DIVISION OF MOLECULAR SCIENCE

20th November 1967

Dear Dr. Shapiro,

Signs of Coupling Constants by Heteronuclear Double Resonance

Tom Connor has suggested that I send a contribution to the Newsletter as a renewal of his subscription and I hope the following note will be of interest to some of your readers.

Saika (I.I.T.N.M.R. 109-18) has discussed the signs of J_{NH} and J_{HH} coupling constants in NH_3, William McFarlane and I have recently performed heteronuclear "tickling" experiments on NH_3D^+ and found that J_{NH} and J_{ND} are of opposite sign to J_{HD}. Since CH_4 and NH_4^+ are both tetrahedral and isoelectronic and in view of the fact that J_{HH} CH_4 = 12.4 c/s and J_{HH} NH_4^+ = J_{DH} NH_3D^+ x γ_H/γ_D = 11.1 c/s, it seems likely that they will have the same sign and since geminal H-H coupling constants in ethane derivatives are known to be negative, we assign a positive value to $J_{14_{NH}}$. The values of the reduced coupling constants ($K_{AB} = 2\pi J_{AB}/\hbar\gamma_A\gamma_B$) are

$$K_{NH} = 60.8,\ K_{ND} = 61 \text{ and } K_{HD} = -0.9, \text{ all x } 10^{20}\ cm^{-3}.$$

We have also been engaged upon an experimental programme aimed at determining the relative signs of coupling constants by heteronuclear double resonance techniques The results obtained to date are given in the table. The signs of the coupling constants have been related to one whose absolute sign is known.

Sign of the Reduced Coupling Constant K_{AB} for directly bonded atoms

A \ B	H	C	F
H		+	
C	+	+	-
N	+	+	
F		-	
Si	+	+	-
P	+	+ or -	-
Se	+	-	
Sn		+	
Te		-	
Pt	+		
Hg		+	
Pb		+	

Broadly speaking the wave mechanical predictions have been confirmed. It appears that the more electronegative elements give rise to less positive reduced coupling constants. Thus all determined coupling constants involving directly bound hydrogen are positive, and all involving directly bound fluorine negative.

Yours sincerely,

Ron Dean.

RON DEAN

College of Arts and Sciences

STATE UNIVERSITY OF NEW YORK AT BUFFALO

Formerly The University of Buffalo, Founded 1846

Department of Chemistry

Acheson Hall
Chemistry Road
Buffalo, New York 14214
Telephone 831 - 3014
Area Code 716

November 22, 1967

Dr. Bernard L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Dr. Shapiro:

In this, the age of computers, it has become prudent to use the complete lineshape equation in analysis of n.m.r. data for rates of chemical exchange. The experimental and theoretical spectral differences are usually minimized by assigning values to the parameters representing the transverse relaxation times in absence of exchange, the chemical shift, the relative population of the sites, and then iterating about a guessed total rate, holding the former parameters constant. I have performed similar calculations on a system with two uncoupled exchanging sites, and have found it also possible to iterate about guessed values for the chemical shift and population parameters as well as the rate for cases involving two distinct peaks, or two peaks close to collapse. I have developed a program ITEREX which performs this feat by a cycle of successive approximations iterating rate, chemical shift, and relative population in that order. It is found that five complete cycles are usually enough to arrive at relatively constant values. The final values of the iterated parameters were found to be independent of the size of the initial guesses.

I found the iterative procuedure for total rate used in the program CURVE4 supplied by Dr. J. Jonas of the University of Illinois most economical, and have used this method in ITEREX. For cases involving one collapsed peak, CURVE4 is most suitable.

ITEREX is written in FORTRAN IV for our I.B.M. 7044-CALCOMP 470 system. Execution time is 46 seconds for five complete cycles per set of data. Documentation is available.

Sincerely yours,

Gareth Templeman

Gareth Templeman

BRYN MAWR COLLEGE
BRYN MAWR, PENNSYLVANIA 19010, USA
DEPARTMENT OF CHEMISTRY
TEL: (215) LA 5-1000

4 December 1967

Prof. B. L. Shapiro
Department of Chemistry
Stanford University
Stanford CA 94305

Dear Barry:

9TH ENC

EXPERIMENTAL NMR CONFERENCE

The ninth Experimental NMR Conference (9th ENC) will be held Thursday 29 February - Saturday 2 March 1968, at the Mellon Institute in Pittsburgh, Pennsylvania. The Conference is devoted to new developments in advanced instrumentation and experimental techniques. It is not a Workshop offering an introduction to the field of NMR.

Sessions will consist largely of invited papers. A limited number of contributed papers may be accepted; manuscripts and applications should be sent to the appropriate Session Chairmen or to the Conference Chairman. Session chairmen will assign the length of invited and contributed papers, and will disperse instructions to their participants. Abstracts MUST be received by Session Chairmen by 15 January 1968 for inclusion in the printed program.

The following are the sessions planned with their chairmen:

A. Allerhand Johns Hopkins Univ. Baltimore MD 21218	Pulse Techniques
D. Anderson Res. & Engr. Lab. Hanover, New Hampshire 03755	Surface Phenomena studied by nmr
P. Bender Univ. of Wisconsin Madison WI 53706	Instructional Techniques
O. Jardetzky Dept. Biophys. & Pharm. Merck, Sharp & Dohme Rahway NJ 07065	Biological Applications

P. Lauterbur SUNY at Stony Brook Stony Brook NY 11790	Less Receptive Nuclei
T. Lusebrink Allied Chemical Corp. PO Box 405 Morristown NJ 07960	Computer-Spectrometer Interfacing
S. Manatt Jet Propulsion Labs. Pasadena CA 91103	Multiple Resonance
L. Snyder Bell Telephone Labs Murray Hill NJ 07971	Oriented Molecules

Additional information, plus an application to attend, may be obtained from the Secretary-Treasurer by responding to the address shown above; those wishing to attend are asked to respond immediately. It may be necessary to limit attendance because of the restriction of physical facilities.

Sincerely yours,

Jay

Jay Martin Anderson
Secretary-Treasurer, 9th ENC
for the Committee:
P. R. Shafer, chairman
E. D. Becker
J. B. Stothers
S. Castellano

UNIVERSITY OF KENTUCKY
LEXINGTON, KENTUCKY

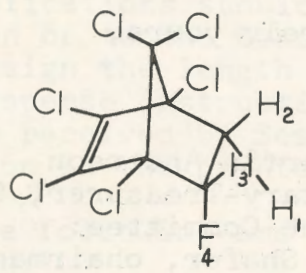
COLLEGE OF ARTS AND SCIENCES
DEPARTMENT OF CHEMISTRY

December 4, 1967

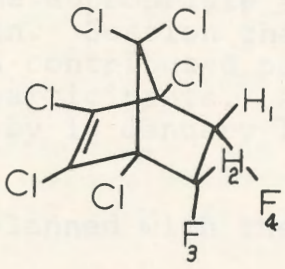
Professor B.L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Barry:

Having examined solvent effects on a series of fluoroethylenes, a study of the Diels Alder adducts of hexachlorocyclopentadiene (compounds A and B) with vinyl fluoride and cis 1,2-difluoroethylene was a logical extension of our previous work. These sp^3 hybridized systems show solvent effects similar to those encountered in sp^2 hybridized compounds.



A



B

Since the effect of temperature upon HF couplings in rigid sp^3 hybridized systems has received little attention, this phenomenon was also examined. Tables I and II list typical results (for A and B respectively).

Table I*

	Temp	J_{12}	J_{13}	J_{23}	J_{14}	J_{24}	J_{34}
Cyclohexane $-d_{12}$	25°C	-13.33	1.83	7.19	25.01	11.92	54.37
$CDCl_3$	25	-13.53	1.81	7.19	25.44	12.25	54.24
$CDCl_3$	70	-13.53	1.80	7.20	25.37	12.19	54.27
CD_2Cl_2	25	-13.66	1.79	7.20	25.66	12.34	53.90
CD_2Cl_2	70	-13.60	1.84	7.18	25.51	12.31	54.26
Acetone $-d_6$	25	-13.88	1.76	7.23	25.99	12.65	53.87
Acetone $-d_6$	70	-13.77	1.80	7.20	25.81	12.53	53.97
DMSO $-d_6$	25	-13.93	1.74	7.19	26.50	13.13	53.51
Δ DMSO $-d_6$ $-C_6D_{12}$		- 0.60	0.09	--	1.49	1.21	-0.86

Table II*

	Temp	J_{12}	$J_{13} = J_{24}$	$J_{14} = J_{23}$	J_{34}
Cyclohexane $-d_{12}$	25°C	6.02	1.84	52.23	16.05
Benzene $-d_6$	25	6.00	1.95	51.86	15.82
Benzene $-d_6$	70	6.01	1.95	51.98	16.57
CH_2Cl_2	25	6.00	1.99	51.86	16.39
Acetone $-d_6$	25	6.03	2.00	51.22	17.06
Acetone $-d_6$	70	6.01	2.03	51.36	17.69
DMSO $-d_6$	25	6.01	2.10	50.77	15.55
Δ DMSO $-d_6$ $-C_6D_{12}$		--	0.26	1.46	-0.50

* Concentration of all samples was 5M%

Preliminary study indicates that the small temperature effect upon H-F and geminal H-H couplings parallels the change of solvent dielectric constant with temperature. As expected F-F couplings show large temperature effects indicative of different coupling mechanisms and solvent-solute interactions.

Geminal H-H and H-F couplings exhibited negative changes in going from low dielectric constants solvents to high dielectric constant solvents. Since the molecular dipole is oriented away from the hydrogen and fluorine atoms, the negative change is in accord with previously observed results.

Yours truly,

Arthur M. Ihrig

Stanford L. Smith

CALIFORNIA STATE COLLEGE AT LOS ANGELES

Department of Chemistry

5151 State College Drive, Los Angeles, California 90032
(San Bernardino and Long Beach Freeways Interchange)

December 4, 1967

Dr. Barry Shapiro
Department of Chemistry
Stanford University
Stanford, California

Subject: Mg(II) Hydration Number in Water-Acetone Mixtures

Dear Barry:

Recently (J. Chem. Phys., 47, 1554 (1967)) we demonstrated that at low temperatures separate proton resonance signals could be observed for bulk water molecules and water molecules in the solvation shell of Al (III), Be (II), Ga (III) and other ions. The proton resonance spectrum in Figure 1 is that of a $Mg(ClO_4)_2$ solution in a water-acetone mixture. Notice separate resonance signals are observed for bulk water and water in the Mg (II) solvation shell. Integration of this and other similar spectra gave a coordination number of six for Mg (II). Thus, it would seem reasonable to conclude that in pure water, as in these acetone mixtures, there are six water molecules in the Mg (II) solvation shell. This result disagrees with the value of four determined by Swift and Sayre (J. Chem. Phys., 44, 3567 (1966)) by a line width technique and it implies that the criticism of this line width method (S. Meiboom, J. Chem. Phys., 46, 410 (1967)) is probably well-founded. Manuscripts describing additional coordination number data for Mg (II) and many other diamagnetic ions are presently in press, and will be sent to anyone requesting them.

Sincerely yours,

Tony

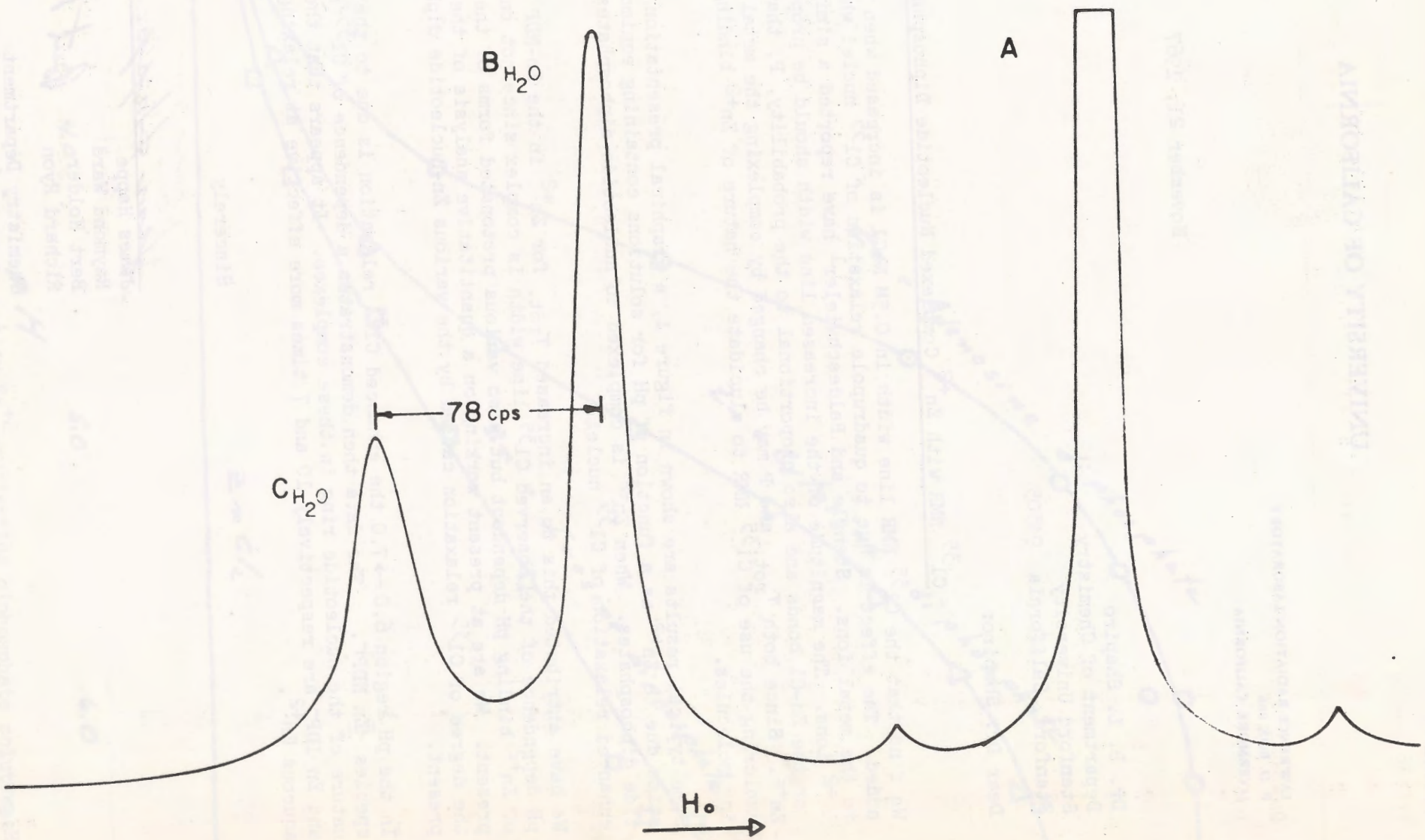
Anthony Fratiello
Associate Professor

Robert Lee
Robert Lee
Vone Nishida
V. Nishida
Ronald Schuster
Ronald Schuster

AF/mk

0.50 M $Mg(ClO_4)_2$ in 1 H_2O: 2 Acetone

T = -81°C



UNIVERSITY OF CALIFORNIA

LAWRENCE RADIATION LABORATORY
P. O. BOX 808
LIVERMORE, CALIFORNIA

November 21, 1967

Dr. B. L. Shapiro
Department of Chemistry
Stanford University
Stanford, California 94305

Dear Dr. Shapiro:

Cl^{35} NMR with Zn^{+2} Complexed Nucleotide Diphosphates

We find that the Cl^{35} NMR line width in 0.5M NaCl is increased when millimolar Zn^{+2} is added. The effect is due to quadrupole relaxation of Cl^{35} nuclei when they are bound to the metal ions. Stengle and Baldeschwieler[1] have reported a similar effect using Ni^{+2} ions. The magnitude of the increased line width should be proportional to $\tau_{rot.}$ for the Zn-Cl bonds and also proportional to the probability, P, that Cl^- is bound to Zn^{+2}. Since both $\tau_{rot.}$ and P may be changed by complexing the metal ions, we have been exploring the use of Cl^{35} NMR to elucidate the nature of Zn^{+2} binding to various complexing molecules.

Some typical results are shown in figure 1, a graphical presentation of the Cl^{35} relaxation due to Zn^{+2} as a function of pH for solutions containing equimolar Zn^{+2} and nucleotide diphosphates. When Zn^{+2} is complexed to nucleotide diphosphates it produces an enhanced relaxation of Cl^{35} nuclei.

We have attributed this to an increased $\tau_{rot.}$ for Zn^{+2} in the Zn-NDP complexes. The pH dependence of the observed Cl^{35} line width is complex since not only is the degree of Zn^{+2} binding pH dependent but also various protonated forms of the complexes are present. We are at present working on a quantitative analysis of the data to define the degree of Cl^{35} relaxation caused by the various Zn-nucleotide diphosphate species present.

In the pH region 6.0 → 7.0 the enhanced Cl^{35} relaxation is due to the unprotonated species $[Zn\ NDP]^-$. The data then demonstrates a dependence of Cl^{35} relaxation on the nature of the nucleotide ring in these complexes. It appears that the species Zn ADP^- and Zn IDP^- are respectively 10 and 7 times more effective at relaxing Cl^{35} than is aqueous Zn^{+2}.

Sincerely

Jim Happe

James Happe
Raymond Ward
Bert Holder
Richard Ryon

Bert Holder

Chemistry Department

JH:gw

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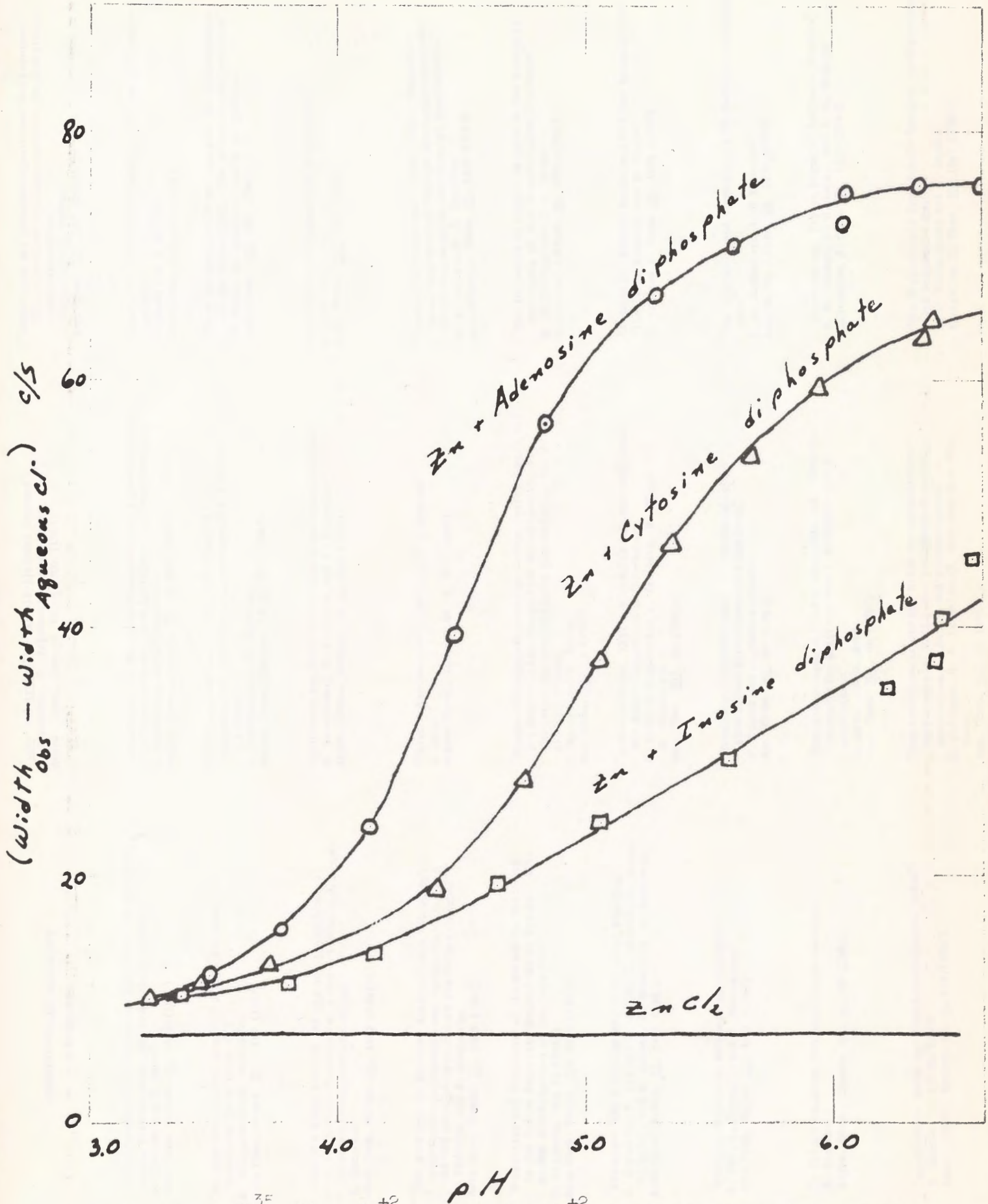

Broadening of Cl^{35} NMR by Zn^{+2} in equimolar Zn^{+2}-nucleotide diphosphate solutions as a function of pH; NaCl = 0.9M; Zn^{+2} = 4.8 x 10^{-3}M.

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