

INTRODUCTION: This E.S. (Emeritus Scientist) is engaged in research activities at the North Eastern Hill University and the nature of the work had been to improve the basis of induced field calculations to be graspable enough entirely over all distant ranges and magnitudes of contributions to the induced fields at a site. This is mainly to enable the interpretation of the Chemical shift values measured from NMR spectra on the basis of simple visualizations and logical deductions. While pursuing these efforts at the calculation methods, it became apparent that, to be able to keep abreast with the fast growing experimental techniques, it is essential to initiate an effort to reinforce the facilities which were being made available at the university as a matter of course with emphasis on instrumentation and computer facilities for data base handling, data processing and computing for evaluating equations. It was heartening that a CSIR project was sanctioned and could be implemented during the three year term from 01-01-2002 to 31-12-2004. That all these efforts have a bearing on "HR PMR Experiment and Theory" would be borne out by the webpage documentation at http://www.angelfire.com/art3/saravamudhan/iitm_crsi_ismar_ca98.html

The text of this proposal consists of **four sections: Section 1:** (1 page) A description of the context of this proposal. **Section 2:** (3 pages) Justification submitted for extension of earlier proposal. **Section 3:** (5pages) An explanation of the observations reported earlier in the contexts of the (a) Advanced NMR Instruments available at High Field (b) Construction of the MASS probe to be completed (c) All the efforts of this PI in evolving a simple procedure for calculations of induced fields in the contexts of magnetic resonance parameters. And, **Section 4:** (1 page) an outlook envisaging consequences and implications to chemistry, physics and biology and the graduate level teaching programs and curricular developments

Section 1: A description of the context of this proposal.

This Project proposal for Grant is to be considered as a sequel to the implementation of the CSIR project entitled: *"Shielding Parameters of Nuclei: Facilities for the Theoretical Calculation and Experimental Determination for Information on Crystal Structures and Molecular Electronic Structures"* at the North Eastern Hill University, Shillong. Only a modest progress could be made on the envisaged objectives by the end of the three year term of the project on 31-12-2004. Since acquiring experience is essential in implementing such projects in an institution where only a beginning has been made, to know the advances in the research area and the techniques which cover the topic of the research project as above, the reports produced by the P.I. in connection with the Research Scheme could be revealing as to what the further course of action should be. Efforts were made to seek facilities from other institutions as and when required: when, the facilities in the host institution, North Eastern Hill University, were not adequate. Enough details were furnished both to the host institution as well as the funding agency CSIR, appraising the necessities for collaborative efforts with other institutions. It was the purpose in such exercises that the funding agencies and the host institutions should be well informed to ensure that the topic of research is pursued in the host institution; instead of the PI getting all the initiatives and efforts to be transferred to some other alternative institution, with the remark that the support in host institution is totally inadequate for pursuing such exercises. Such a reaction would not be progressive for imparting knowledge in a location where, probably as a conjecture, the prevailing situation is such that the advantages of a growing technique remains unreachable; that too, to such an extent that there would be no initiatives or support even if there could be advantages that can accrue because of this research activity. In the present case of the CSIR Research Project No: 01/1767/ (02) EMR-II, what was the appreciation of the funding agency and the host institution remains oblivious to the PI since the request for an extension did not get an approval. It is the sincere assessment of the P.I., hereby reporting that an effort must be made to secure and instill interest in the subject matter of Magnetic Resonance in this location with even greater vigor lest when the host institution develops the educational activities, sooner than later, it would become obvious that there had been an imbalance in the growth and would not be easy to make amends for not reinforcing this area (Magnetic Resonance) of research to develop and grow at the right time. All the required report materials that would be useful in assessing the context have been made available by the PI in the following [URL built](http://www.saravamudhan.tripod.com/csir_schm_sa/) by the PI exclusively for the purpose of documenting the progress made in the project. URL: http://www.saravamudhan.tripod.com/csir_schm_sa/. Ever since that project was sanctioned, and, the implementation of the project began; there have also been significant changes in the basic infrastructure available at the Host Institution N.E.H.U. While such changes took place it was also found necessary to discern the following: *whether proper cognizance prevailed that an approved research project has been going on, and, whether the present state of the infra structure available is an improvement over what was available.* But, the answer to such concerned queries is all a matter that which is at the moment beyond the perception and appreciation of the PI. And, knowing about these factors for the actualities would definitely promote the interests in the growth of Magnetic Resonance.

SECTION 2: To elaborate on the Context of this Proposal, the justification (text below with 3 sections) submitted for the extension of an earlier proposal is included herewith without modification: The extension applied for earlier was not approved.

2.1 The Following points indicate the DEVIATIONS from the nature of the original plan of work and require more support from the External Agency to be pursued after the Termination of the Scheme (01-01-2002 – 31-12-2004).

The first phase of the project implementation as envisaged in the original research proposal was to construct the Magic Angle Spinning [MAS] Probe for the AC 300 NMR Spectrometer at the RSIC, NEHU for which it was planned to collaborate with NCL, PUNE. There had been neither change in this prime objective to provide the MAS facility nor any change in the requirement of the collaborative effort.

However there had been a change in the methodology and the materials due to the following turn of events:

1. The main component for the construction of MAS assembly is the stator/rotor assembly and this part of it was supposed to have been a stock available at NCL as much as it was used for the previously published MAS construction. Soon after the CSIR Scheme of this PI at NEHU was sanctioned [by this time this was all efforts of two-year-before 01-01-2002] the situation prevailing was that the stock of stator/rotor assembly at NCL has become not so much of available material for this purpose and efforts to contact the various manufacturers for procuring the spare part stator/rotor took about 2 months. And promptly replies were received that no manufacturer would be selling this item as listed component except as a spare assembly for their original MAS Probes procured. This situation was a set back but, effort by this PI in trying to contact Bruker BioSpin {Sales/Marketing Division} on this matter resulted in an optimistic turn since the Bruker BioSpin exuded such an understanding in this context that they were making possible for this PI to procure the Bruker's original Mechanical assembly with stator/rotor at the costs amounting to reasonably within the reach of the equipment grant in this Scheme. This scene was neither known before as a possibility, nor it is any compromise of the original plan as portrayable by the descriptions below:

2. The fact at RSIC, NEHU is that the entire maintenance and operational aspects have to be with the available technical assistants at RSIC, who do not have experience in the Solid State NMR aspects either instrumentation or the Magnetic Resonance Technicalities. If a probe constructed entirely indigenously is brought before them, then to make them get used what another user [though it is this PI with reasonably well equipped with the required prerequisites to use and impart training] has to provide on his own Research project [and not a unit procured from the manufacturers well known to them with familiar service personnel] would have been an inexplicable hurdle. This has now turned out to be nonexistent because the mechanical assembly as they would be handling would be the familiar Bruker design like that of the present liquid-state NMR probe setup. No longer there is any requirement for trying to acquire the stator/rotor assembly separately. This is a special offer from Bruker BioSpin for the research project of this PI.

3. These developments could take shape at a much slower rate than what otherwise would have been including the delays of having to go through the acquiring of purchase committee approvals for the required import of this assembly.

The above has the major contribution in changing the course of implementation to this stage. Since the scheme was approved only two years after the first initiatives, at the outset while commencing the scheme on 01-01-2002 the PI had a rather gloomy picture at the time of receiving the sanction of the scheme than this cheerful turn.

That no staff [JRA/SRA/RA] could be appointed in this scheme is a trend quite obvious and explainable, given the experience of this PI during the early stages of the installation and utilization of the facility at this NMR System in NEHU, Shillong. But, this would be the enthusiasm on this project was not in any way a foregone conclusion even though there are reasons to state for this continued nonavailability of technically motivated research scholars. This state of the technical know-how had prompted this PI to set the trends for an "INNOVATIVE PROGRAMME" initiatives on Magnetic Resonance Spectroscopic Techniques. Thus unintended outcome is the drafting of a viable course curriculum and get this also reviewed by the expert committee of the UGC is an unstated outcome of the efforts to implement the CSIR Research Scheme on providing a reinforced Magnetic Resonance Facility at this University.

2.2 The following enumeration, of the Work Done During in the previous scheme, indicates that for the changed Plan of Work and the progress made thus would require a much longer evolution period under the support of the CSIR so that a clear appreciation of the realization of the Objectives emerges, in spite of the changes and how the support from the external agency has contributed necessarily to the advantage of the host institution:

Significant progress has been made in implementing the first phase of the project, namely, the construction of the Magic Angle Sample Spinning MASS probe accessory for the AC 300 NMR Spectrometer at the RSIC, NEHU. The spontaneous special offer from Bruker BioSpin to provide the basic mechanical assembly of the Probe (MASS) body has reduced the effort in acquiring good quality material for the construction of the probe and has it designed and machined in a precision work shop.

During the process of implementing this project, *particularly because of the experiences gained while trying to appoint a staff in the project*, a necessity arose for working out a durable curricular contents for a graduate programmes, appropriate and compatible with the average student level, so as to impart a capability to them to gain the technical know-how for using the Magnetic Resonance Spectroscopy at a rate commensurate with the rapidly advancing technological provisions for the utilization. A considerable progress has been made in this direction, and the course-curricular structure drafted out by this PI under the frame work of the INNOVATIVE PROGRAMME of the University Grants Commission has been reviewed by an Expert committee of the UGC and found adequate for a PG level course on Magnetic Resonance Spectroscopic Technique. However, the PI would be able to surge forward only if a Bench top Nuclear Magnetic Resonance spectrometer Unit could be procured as a supplementary unit to the existing FT NMR AC 300 Spectrometer at the University. This requirement of a durable Syllabus, though was under the consideration since a long time, did gain the necessary emphasis during the course of implementing the CSIR Project. This activity was not explicitly indicated as a specific phase in the objective of the CSIR research proposal. Nevertheless, implicit is that advantages accrued due to the support of the CSIR towards the overall need for improving the infra structure facilities.

This effort would go a long way in trying to impress on the users of the RSIC facility about the MASS technique and its use in effectively extracting structural information on systems which are hitherto being studied only in liquid state NMR. This would be contributing to the lasting benefit of the CSIR Scheme which would continue to accrue even after the termination of the CSIR project. While evolving this course structure, the other explicitly stated phases of the CSIR Schemes have implicitly progressed without a necessity for any chronological sequence to implement the phases in the sequence as listed out in the original research proposal.

The effort to make progress on the results, which were obtained for the NMR measurements made at the TIFR, Mumbai during August 2003 with the VARIAN UNITY 600MHz NMR Spectrometer, have gained in their significance in view of the contributions made by this PI in the National and International Symposia and Conferences on NMR. These trends seem to be further substantiated by what is being currently reported in literature as clarifications on interpretations of chemical shifts and induced fields.

These effectively pave the right way for the use of the MASS facility [phase 1 of the CSIR Research scheme] when the construction is completed for use.

2.3 The following description of the Nature of the work yet to be done should indicate to the Funding External Agency what could really be the credibility that the Funding Agency can look for when this task is accomplished, from the point of view of the what accrued till now due to this CSIR Research Scheme

The electronic components required for the tuning of the sample coil of the MASS probe have to be acquired and it is known now that these have to be imported and are not available as listed items for sale by the manufacturers of the MASS probes. This would require considerable effort to find components available from General Electronic Component suppliers that match the specifications of component as required for a specialized instrument like MASS probe.

There are several aspects of the present FT NMR Spectrometer System [the AC 300 at RSIC, NEHU] which have to be looked into since only on the basis of the Working AC 300 system, the constructed probe would become useful. Or else CSIR may have to find an alternative placement for this MASS probe unit if its construction is completed since the cost of this import item exceeds Rs. 3 lakhs. This may not be a difficult task since this is a collaborative effort with NCL, Pune where there are requirements for probes of this type and where there are several FT NMR systems already functional.

As listed out in the last page of the Website URL: http://saravamudhan.tripod.com/csir_schm_sa/ it is essential to procure software packages which are for structure-prediction-types based on chemical shift data. Thus the packages are essentially (i) Data bases of known spectra and chemical shifts (ii) packages enabling calculation of Chemical shifts of nuclei in molecules using theoretical procedures. Acquiring of these packages would require

utilization of funds under appropriate head of accounts. The project originally submitted did not include the cost of these soft wares since as originally intended if a staff could have been appointed, the scholar would have had to spend the time in exclusively the first phase of the work since this requires acquiring skills in electronic instrumentation aspects which is not imparted as a matter of routine in the regular PG level curriculum. Since the effort to attend to the training of a staff was absent, the PI could spend time on the effort to look out for software packages which meet the specifications to be handled by, technical assistants to start with to the extent of maintaining PCs and Workstations supporting these soft wares as part of the facility and let the qualified assigned users to avail these software facilities. Since it is possible to find scientists handling such soft wares near this Centre for their requirements making this as a facility part of NMR facility in a University is a different trend which requires more efforts knowing the specialized package capabilities and the user environments which would enable the use of the same.

Acquiring data from Spectrometer on to another PC which is not a part of the spectrometer system of the manufacturers and processing data is a trend which requires unconventional efforts and from the displays in the Conference pavilions and other resources, reinforcements have to be added which would take shape when the first phase has been completed and the MASS probe accessory is functional.

The work which is being presented by this PI on INDUCED FIELD Calculations pertaining to magnetic moments and their effectiveness in explaining the trends of observed chemical shifts [<http://saravamudhan.tripod.com>], has certain relevance for the MASS techniques. Particularly, while this PI was indicating the possible applications of these calculations in biological cells with different susceptibilities inside (inner compartments) and outside (outer compartments) the cell, these indications are being substantiated as valid by some of the recent publications in the Journal "Magnetic Resonance in Medicine" {Vol 51, Number 3, page 441, March 2004} and "Concepts in Magnetic Resonance" [Vol 18, pages 72-95, 2003]. This encouraging trend has to be reinforced by this PIs intended trend of experiments [see the results reported in the webpage cited above, particularly the spectra with capillary tubes inside a 5mm NMR tubes]. The collaborating Scientist at NCL had expressed interest in experiments which this PI had been envisaging on magic angle spinning of liquid state samples for their consequences which are not very far from what was being reported currently in leading journals.

The present state of the PIs concerns on Induced Field effects and the Lorentz ellipsoids/spheres can be appreciated by the documentation at the URL: http://geocities.com/saravamudhan1944/eenc_ampere_lille.html and the other links to web pages in that Webpage.

All these at present which this PI has indicated can be realized by this PI only if the supportive measures to promote such interests are reinforcingly enhanced. However, along these indicated trends any appointed staff can be trained and with assistance from resource persons at National NMR facilities in this country, the work can be constructively progressing. Hence it all depends on the Host institutions' appreciation of the purposes and the invigoration by the Supporting external agencies, in the cause of making this institution as part of the national stream. This coordination of the activities at this RSIC, with the National Facilities at TIFR, Mumbai and IISC., Bangalore is what is to be aspired as a durable consequence of this CSIR Scheme at NEHU with the collaboration of NCL, PUNE.

More details would be possible in the Final Technical Report soon after the 31st December 2004. Hence this PI would reinforce further the requirement of an Extension for this Scheme by one more year by trying to have a Plain paper application duly forwarded to CSIR by the Head of Institution.

The provision of providing a durable curricular training on the spectroscopic techniques based on Magnetic Resonance phenomena would surge forward if the Rs. 42 Lakhs required for the bench top models could be forthcoming as the Extra Equipment Grant. As an alternative the PI for this purpose should be requisitioning by a renewed application this amount from the Rs 50 lakhs set forth as possible grants by UGC for purposes of the INNOVATIVE PROGRAMMES. An OUTPUT DATA to UGC in the prescribed form would be sent indicating the situation by this PI as a provisional measure for an approval to be sought as coordinator of the envisaged programme.

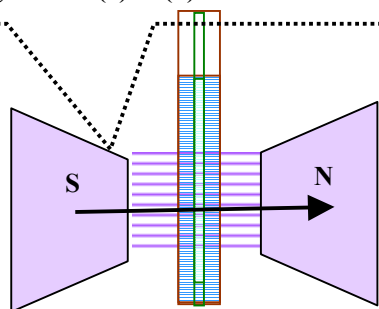
Even though all the amounts sanctioned under the project were not released, and, the Extension of the Term of this CSIR project (applied for by the P.I. was not approved, it has been possible to continue the work beyond the TERM (after 31-12-2004) since the funds which remained unutilized during the regular term of the project was made available to the P.I. to incur the necessary expenses.

Section 3: An explanation of the observations reported earlier (*reference cited on page-7 of this proposal*) in the contexts of the (a) Advanced NMR Instruments available at High Field (b) Construction of the MASS probe to be completed (c) All the efforts of this PI in evolving a simple procedure for calculations of induced fields in the contexts of magnetic resonance parameters (page# 5 to9)

FASS Probes: Fixed Angle Sample

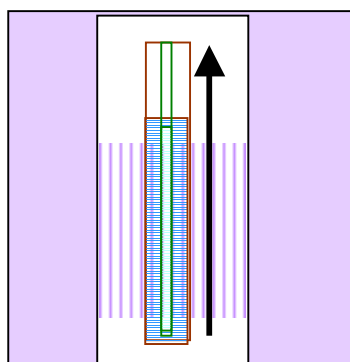
spinning probes:

Only perpendicular-to-the-magnetic field
Configurations (a) & (b) below



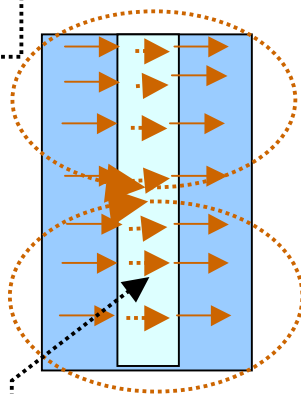
FASS coils: (a)

Electro Magnet Systems and Permanent Magnets:
(up to 100Mhz Proton NMR frequency)



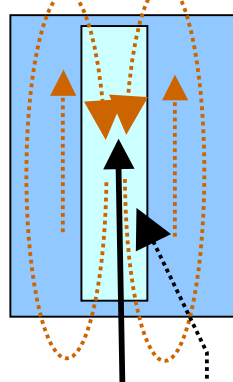
FASS Coils (b)

Superconducting [Supercon]
Magnet Systems : 200 MHz
and onwards up to currently
highest value of 900 MHz
proton NMR frequency



Field at the inner
capillary water

Applied field + the
induced field
FASS (a)

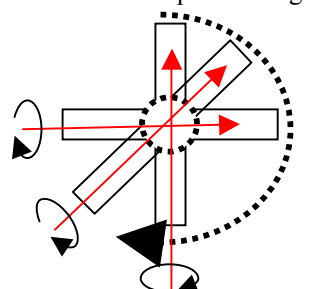
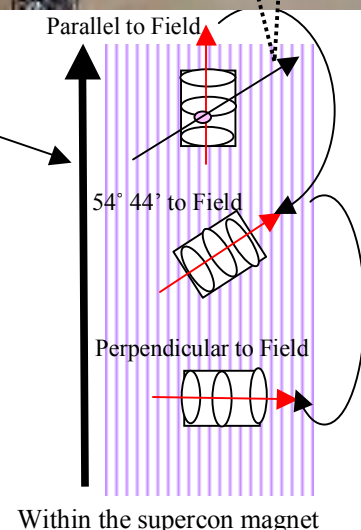
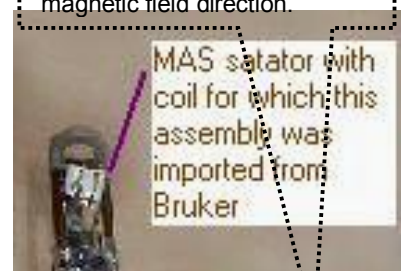


Field at the inner
Capillary water

Applied field - the induced
field **FASS (b)**

VASS Probes: Variable Angle Sample Spinning Probes.

By construction in these probes the sample can be inside a coil whose solenoidal axis can be changed in orientation from Parallel to the magnetic field gradually to perpendicular to the field. Mostly the probe heads for Supercon Systems have the MAS versions. Below is an illustration of how the same coil can be rotated to have different angles with magnetic field direction.



$$h\nu_{\text{Res}} = g\beta H_{\text{Res}}$$

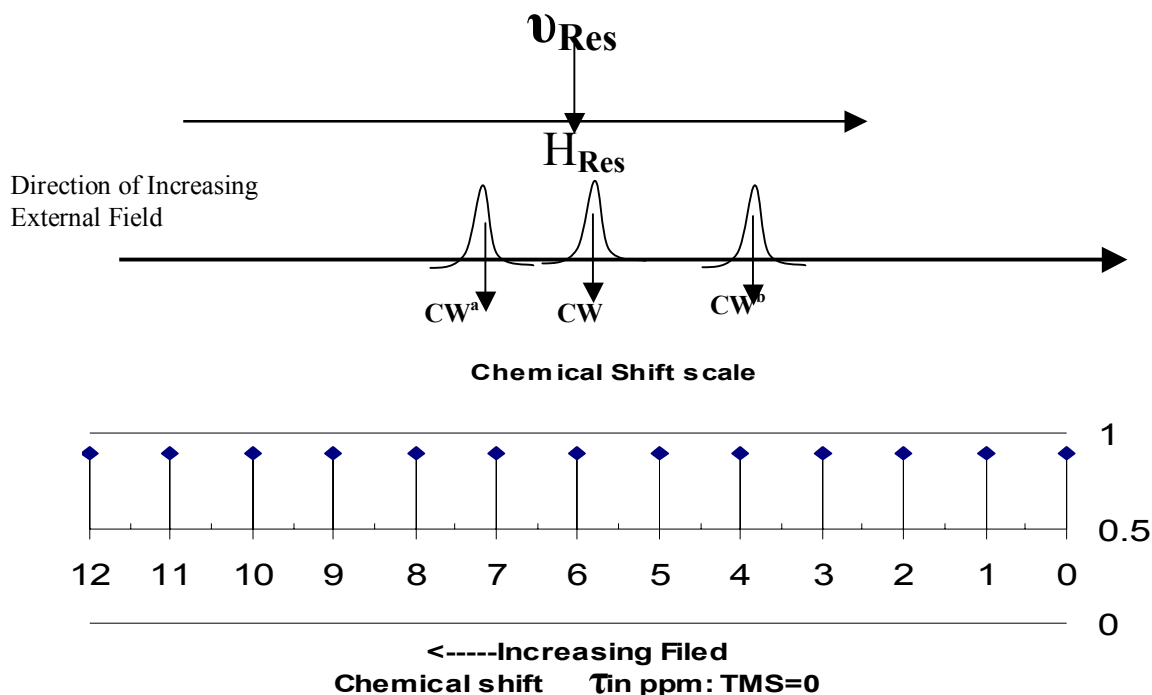
ν_{Res} = Resonance Frequency is held fixed. [Consider the Resonance of Capillary water for different contents in the outer tube surrounding that capillary.

H_{CW} stands for the resonance field for the Capillary Water when no paramagnetic material is placed in the outer tube. This means $H_{\text{Res}} = H_{\text{CW}}$

For FASS (a) the induced field [due to the paramagnetic substance in the outer tube] adds to the Field experienced by the Capillary Water. Hence the field at Capillary would be more than what the value was without paramagnetic substance:

$$H_{\text{CW}}^{\text{a}} = H_{\text{CW}} + \Delta H^{\text{a}}_{\text{induced}}$$

That is $H_{\text{CW}}^{\text{a}} > H_{\text{CW}}$; this would require externally adding a field “ $-\Delta H^{\text{a}}_{\text{induced}}$ ” to bring the field at the capillary to the required resonance value for ν_{Res} . Or as the field value is slowly scanned near resonance, the resonance can be observed only at an external field value lower than the previous filed value.
CW

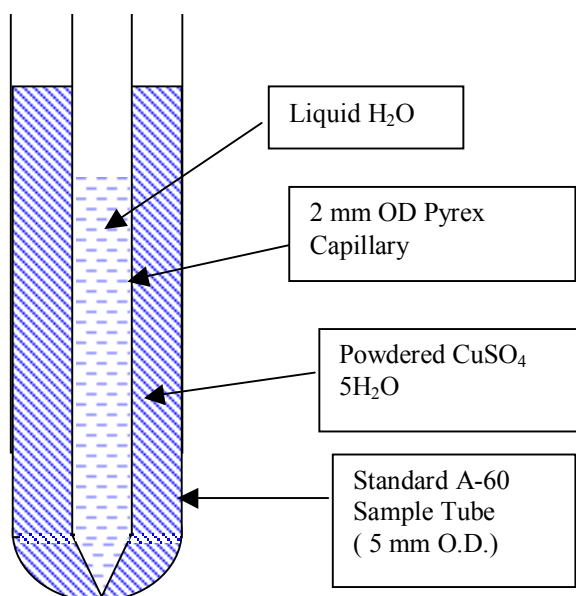


For the context of current efforts of Dr. S. Aravamudhan, a consideration of the NOTE published earlier:

In the Review of Scientific Instruments Vol.37, page 1099 (1966): by Author: **J.Q.Adams**: Title of paper: **Measurement of Static Paramagnetic Susceptibility with High Resolution Proton NMR Spectrometer:**

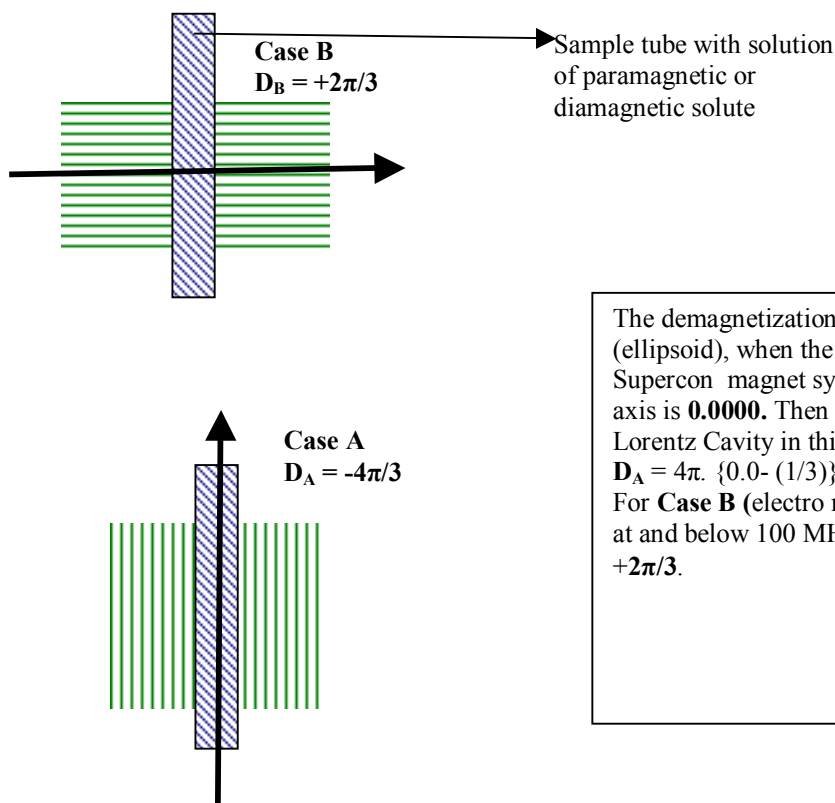
This note has experimental results obtained from an A60 Varian NMR spectrometer.

A60 NMR Spectrometer is of the type which comes under the systems with Electromagnets which can be categorized under the **FASS (a)** probe systems. The author used a sample tube with inner capillary within a sample tube of 5mm OD. When Copper Sulphate penta hydrate powder sample is filled in the outer tube, the water sample inside the capillary recorded a downfield shift (a direction towards the TMS reference) of 90 Hz from the water sample which was not surrounded by Copper Sulphate powder. This was conclusively a 1.5 cgs / Hz of susceptibility value measure for the copper sulphate.



This corresponds to the FASS (a) configuration for the Magnetic Field Direction, Sample coil Axis and the Spinning axis of the sample tube.

For CuCl₂ and CuBr₂ 27.2 x 10⁻⁶ cgs units and 14.1 x 10⁻⁶ cgs units are the volume susceptibility values measured with respect to CuSO₄ 5H₂O by these experiments.



The demagnetization factor, for an infinitely long cylinder (ellipsoid), when the field is applied parallel [Case A ; Supercon magnet systems above 100 MHz] to the cylinder axis is **0.0000**. Then the effective Demagnetization inside a Lorentz Cavity in this sample would be $D_A = 4\pi \cdot \{0.0 - (1/3)\} = -4\pi/3$. For Case B (electro magnet or permanent magnet systems at and below 100 MHz), $D_B = 4\pi \cdot \{1/2 - 1/3\} = 4\pi/6 = +2\pi/3$.

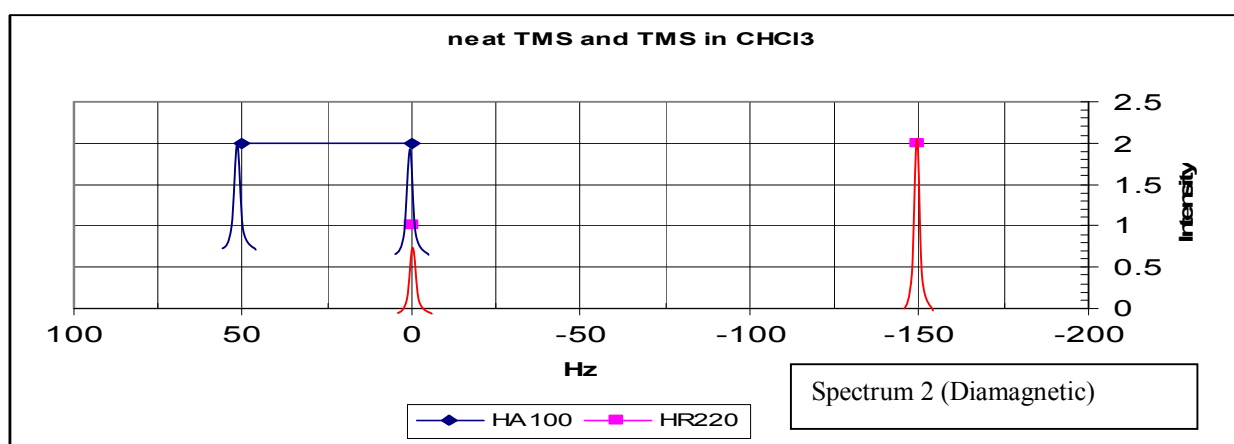
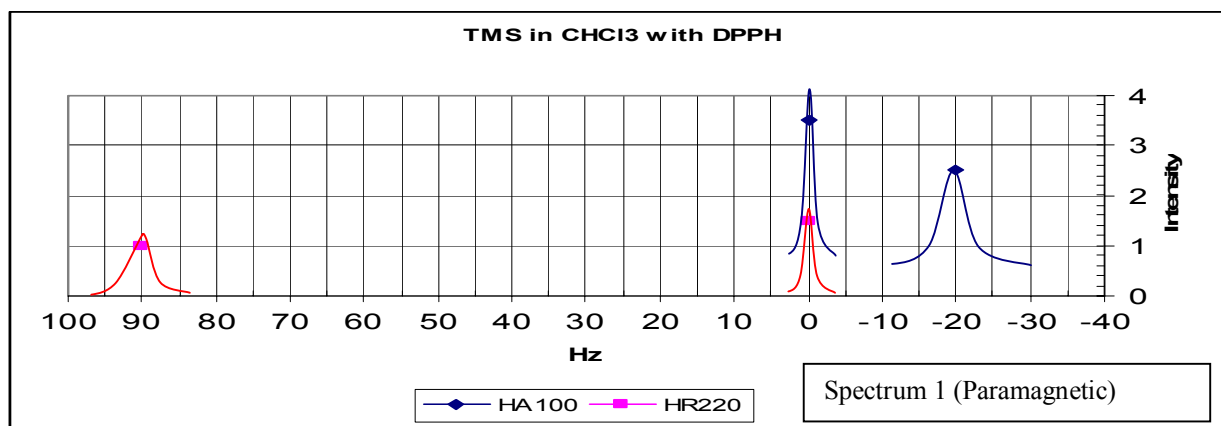
For Paramagnetic Samples the Susceptibility values are +ve and for diamagnetic samples the susceptibility values are -ve. This implies that the induced fields will be along the direction of the external magnetic field for paramagnetic systems. For purposes of NMR the shifts are measured with respect to a reference and the correction is given by $\delta_{A,B} = D_{A,B} \{\chi^{\text{ref}} - \chi^{\text{sample}}\}$. The χ^{ref} is for the diamagnetic (-ve susceptibility values << paramagnetic +ve Susceptibility values) substance inside the capillary. Hence for a DPPH solution (paramagnetic) δ_A will be negative and hence downfield from reference; δ_B will be positive and up field to the reference peak.

A careful scrutiny of this situation would indicate the differences from the induced fields within a capillary of pure liquid inside this solution in the sample tube. These points as above are to be appreciated for explaining the experimental measurements reported in the article entitled: "*Bulk Susceptibility Corrections in Nuclear magnetic Resonance Experiments Using Superconducting Solenoids*" by D.Live and S.I.Chan, **Analytical Chemistry**, Vol.42, No.7, pages 791 &792 (1970).

Relevance of the above descriptions on demagnetization effects can be found at the following URLs of this E.S.

<http://nehuacin.tripod.com/id3.html>

http://nehuacin.tripod.com/pre_euromar_compilation/



Spectrum 1: TMS+CHCl₃ Solution in Capillary within 5mm Sample tube containing DPPH free radical (paramagnetic) solution in TMS+CHCl₃. Reference '0' set for the capillary proton signal. Blue HA-100 Case B. Red HR220 Case A.

Spectrum 2: Neat TMS reference (set to '0' ppm shift) in capillary and TMS + CHCl₃ (more diamagnetic than neat TMS) in the sample tube. Blue HA-100 Case B. red HR-220 Case A.

The spectra till now obtained at several institutions where FT NMR facilities are available indicate that an extra effort has to be put in to setup the spectrometer conditions for acquisition of spectra in the absence of a deuterium signal to secure a field frequency lock. In most of the spectrometers (Bruker, 200,300. Jeol 400Mhz, 60MHz and Varian 600MHz, 400MHz, 90MHz) the spectra could be acquired without field frequency locking. The required trends for the shifts due to paramagnetic outer sample could be observed for a inner capillary water sample using the standard 5mm NMR sample tubes. This preliminary effort was necessary because the first observation of this type was reported with one of the early Varian A60 spectrometer and subsequently with 100MHz and 200MHz spectrometers. The usage of the possible variation of angles with VASS probes is a significant feature in this proposal. The induced field calculations reported by this author in various conference/symposia till now by this author would require a few experiments to be carried out to prove its utility and applications in the context of NMR. <http://nehuacin.tripod.com/id1.html>

SECTION 4: An outlook for the future trends of this research proposal

Line Shapes in Magnetic Resonance and the Average Static Magnetic Field at a Site: The Role of Discreteness and Continuum within the Material

When there are no time averaged fields (1) to be accounted for, then, within the materials it is the totality of the static fields at every one of the sites [distributed within the material] which manifests in a magnetic resonance spectrum. This essentially implies the spatial distribution of the static magnetic field which contributes to the line shape. Since the discreteness of the contribution from adjacent sites [to be resulting in a summed up total contribution], depends on the nature of material constituents within a small range of distance compared to the macroscopic extent, this contribution can be obtained as a calculated sum for a typical site within the material, [this can be taken to be the Contribution from within Lorentz Sphere (2)] and further considered to be the same for every one of the sites in a homogeneous medium. But the contribution from the remaining bulk of the material could be much more difficult to track and estimate at each site by the methods known till now (3) particularly when the material has such shapes to be causing inhomogeneous induced field distributions even in a homogeneous medium. The methods, used since early days to calculate demagnetization factors, make evident the kind of complications that arise in estimating induced fields within material specimen of arbitrary shapes. All these complications in estimating the induced field distributions and analyzing the observed patterns in spectra, require stringent experimental conditions for implementing certain techniques for their obvious utilities. The case of HR PMR studies in single crystals for determining molecular shielding tensors is such a complication which required invariably making single crystal spheres from single crystals of every organic molecular systems of interest (4). There have been efforts to devise rapid computational methods to calculate such induced field distributions within materials (5).

It has been possible, since recently, to evolve (6) a simple summation approach to calculate induced fields within a material which can reproduce the known, standard demagnetization factors with comparable accuracy. This method seems capable of simplifying the procedure to estimate the induced fields within the material [and, even outside a magnetized material (7)] and provides a diversion to circumvent the necessities to be considering an “average field” as being represented by the calculated values. This method has been described (8) earlier with an enumeration (9) of the associated advantages. The impact of these results can be effectively enunciated with specific reference to the analysis of line shapes of magnetic resonance spectra of materials.

- (1) W.C.Dickinson, Phys. Rev., **81**, 717 (1951). (2) S.Aravamudhan, Ind. J. Phys., **88**, 985 (2005). (3) G. Mozurkewich, H.I.Ringermacher, and D.I.Bolef, Phys. Rev. B, **20**, 33 (1979)
 (4) http://www.geocities.com/saravamudhan1944/eenc_ampere_lille.html
 (5) P. Vallabh Sharma, Pure Appl. Geophys., **64**, 89 (1966)
 (6) http://nehuacin.tripod.com/pre_euomar_compilation/id7.html
 (7) <http://saravamudhan.tripod.com/id6.html>
 (8) Poster Sheet_7 to Sheet_10 at http://www.geocities.com/inboxnehu_sa/nmrs2005_icmrbs.html
 (9) Sheet_11 at http://www.geocities.com/inboxnehu_sa/nmrs2005_icmrbs.html

This PI has contributed to the National symposia of Indian Biophysical Society and International Biophysics Congresses where in the possible applications of Chemical shift Tensors (aromatic ring current shifts) and the Induced Fields in the context of paramagnetic shift reagents in MRI experiments have been considered. The PI has published to the Internet an article on NMR entitled: NMR as a Tool for Structure Determination which can be displayed at the URL: http://www.geocities.com/saravamudhan2002/nmr_article.html. In addition a consideration of the NMR techniques in the context of standardizing the medicinal plants and an initiative would be made to contribute an appropriate article on the use of solid state NMR techniques:

http://www.geocities.com/inboxnehu_sa/Proj_bicnehu.html. A progress is being made to envisage curricular requirements for facilitating an appreciation of advanced aspects of Magnetic Resonance in early enough stages of the post graduate level courses http://www.geocities.com/saravamudhan1944/ugc_inno_proposal.html

http://www.geocities.com/inboxnehu_sa/conference_events_2005.html
http://www.geocities.com/inboxnehu_sa/conference_events_2006.html