

2.[a] Impact Teaching(page-2-)/Research(page-3-onwards)

http://aravamudhan-s.ucoz.com/saravamudhan44/ugc_inno_proposal_m.html

3. Specify objectives and goal to be achieved, with its impact on teaching, research or both.

As specified in the (may be found enclosed) Attached Additional Sheet AAS # 1

[CLICK HERE to download AAS#1](#)

AAS #1

Magnetic Resonance Phenomena provides a unique context for understanding the application of Quantum Mechanical Formalisms with the spin Hamiltonians and the spin-state wave functions since the early descriptions of the phenomena can be introduced with classical vector pictures and equations obtainable from the considerations of motions of classical bodies and magnets. The specific reasons - as to where and why the quantum mechanical descriptions become inevitable - throw a great deal of light into the realms of applicability of quantum and classical descriptions.

The mathematical prerequisites are much more elementary than what the students usually contend it to be and it is necessary, at least in the case of students who specifically seem to hold the bias of not opting for mathematics, but opt for subjects which do not titled explicitly in mathematical terms. This trend leads them invariably to the ordeal of trying to use much less straightforward approach while having to apply mathematical procedures, which learnt, as a revision of elementary level mathematics would be much simpler.

This required **elementary revision**, (even though a few talented teachers can venture into), **finds obviously, a description** as follows. That, it is a strange way of handling the subject matter and not many in such contexts seem capable of supporting since magnetic resonance itself is a much more recent and advanced technique which is being encapsulated for application without having to learn too much about the phenomena and its descriptions. This usefulness makes the students not well appreciate what they are not able to use of this technique. Hence an exclusive effort of the sort of innovative program is worth giving a try at the North Eastern Hill University, Shillong

Magnetic Resonance Phenomena provides a unique context for understanding the application of Quantum Mechanical Formalisms with the spin Hamiltonians and the spin-state wave functions since the early descriptions of the phenomena can be introduced with classical vector pictures and equations obtainable from the considerations of motions of classical bodies and magnets.

[CLICK HERE to download AAS#4](#)

AAS #4

This is an effort in trying to illustrate that what is being considered as a stringent requirement and formidable. For the students with **insufficient background it can possibly be made simpler, and show that what is required is a simple revision of elementary aspects** already taught at lower levels but are not covered at all the intermediate levels with the required emphasis on revision since the main title gets importance only at relatively higher level of the Curriculum.

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 comptible 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. Aconsiderable 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.

http://sravamudhan.tripod.com/csir_schm_sa/id24.html

“Magnetic Resonance Phenomena provides a unique context for understanding the application of Quantum Mechanical Formalisms with the spin Hamiltonians and the spin-state wave functions since the early descriptions of the phenomena can be introduced with classical vector pictures and equations obtainable from the considerations of motions of classical bodies and magnets”

1) By Spin-Hamiltonian, the operator form of the Classical angular momentum vectors are to be appreciated. Thus, it is necessary to reemphasize the Classical Vector description and the QM Operator analogues while introducing the Vector Model of the atom while dealing with the atomic structure descriptions in the early stages of QM courses. Most of what is required in the Chemical context (as different in the spectroscopy discussions, Magnetic resonance in particular) is the single spin description of what is coupling of angular moments and what really is meant by interacting angular moments (spin-spin or spin-orbit). By making out a definition from the conventional way the term interaction results in consequences, it must be made clear to the learners that an interaction of the Spin and orbital angular momentum arises because of the inevitably associated magnetic moments related to the angular moments. In addition, the quantization rules are stipulated only in terms of the magnitudes and components of angular moments. The simple fact that the angular momentum magnitudes are related to the associated magnetic moments by well-defined rules, most of is that the angular moments are related to their associated magnetic moments by universal constants of proportionality. Thus, it becomes possible to describe interactions in terms of the angular moments taking for granted the relations available to relate the angular moments with the magnetic moments. This aspect deserves a much greater emphasis in curriculum stipulations and course contents than what is prevailing particularly at the Bachelor's degree levels if not in School curriculum. A persistent effort can bring about a perceptible change in quality when it comes to grasping advances in chemistry, which owes a lot to the way the roles of angular momentum is employed for interpretations. In the context of general chemistry, the single spin descriptions with due importance for not only the conventional z-components, but also what should be the disposition of x, y components with regard to interacting and non-interacting angular moments (Contents of NSC12 http://aravamudhan-s.ucoz.com/symposia_2009_2010.html display Sheets 8 to 12 http://aravamudhan-s.ucoz.com/NSC12_Aravamudhan.doc). Whenever the energy of interactions (for coupled angular moments) is expressed, it should be emphasized that the associated magnetic moment interaction should be evident.

2) As for as spectroscopic discussions are concerned, there must be considerations of ensemble of angular moments / spins, the Magnetization for example as a result of the individual spin moments, and the time evolution of the ensemble property with due awareness of what happens at the individual spin / orbital moment level has to be included to make the subject matter easier at the higher educational levels. Trying to build up the teaching materials from this elementary level while teaching advanced spectroscopic aspects invariably leaves the delivery of the material partial only at several stages, and this causes impediments in the progress both to the teacher and the taught. This led to a conclusion at some stages that leaving the use of the advanced technique to what only gets to know from the prevailing state of the art in particular research group, rather than motivating the users to avail the full potential. This has been resulting in the conflicts that was encountered while teaching chemistry effectively and required an out-of-the-way innovative approach for preparing and teaching materials to find an alternate effective ways, whenever an opportunity enabled the displaying of such materials. This amounted to, at a certain stage, teaching of the subject matter redundant or unnecessary exercise, thus pointing out the importance of trying to find ways and means for effective percolation of the essential requirements to the much earlier stages of education. At the higher levels, such a background can be consolidated by pointing out the advances as mere consequences of the elementary aspects. It gives also ample time while teaching, at advanced levels, to show how the technological progress has aided the understanding of the basic science to the extent of making possible otherwise not so easy experiments.

The current advances in spectroscopic techniques, to be grasped, require ever-growing awareness that experiments are carried out on bulk materials and inferences are as if it is all a reflection of only the presence of a single molecule. The technology has furnished such sensitivity enhancements and expanding for greater details, that this fact about the single-molecule to bulk material and the converse of it must be adequately stressed in the early education levels that it does not require much emphatic mention at the higher levels. Then, curriculum content can be delivered much more effectively as the students' progress from one stage to higher stages. The mention of the state of theory, that mostly it is on isolated molecular procedures unless further developments provide for including the influence of the near neighbors and the bulk continuum. Once again due importance must be attached to the fact that discreteness and continuum within matter gets only a qualitative demarcation; setting quantitative boundary conditions requires a careful assessment of what gets included, and what does not for consideration.

Multiple Pulse HR PMR in solids on Single Crystals of Organic Molecules

Results in the determination of Full Shielding Tensors of Protons in Molecules: Enables the electronic structure elucidations of molecules

Principle: *Shielding is the consequence of induced fields; magnetic secondary fields are induced by the electronic charge circulations; Charge circulations in presence of magnetic field depend on the Susceptibility of molecules to undergo alterations in electronic charge circulation characteristics. Molecular Susceptibility is thus related to the induced fields and chemical shifts. It could be interesting to point out here that the original NMR study is based on a phenomenon related to specifically nuclear magnetism described in terms of nuclear spin properties. The results could provide insight and further indicate possibilities for consequences in bulk magnetism not necessarily described in terms of quantized angular moments, but the ensemble consequences in condensed matter due to the magnetic susceptibility.*

Excerpt from home page: <http://saravamudhan.tripod.com/index.html>

The present subject of research has inception at the instance which made a breakthrough in the explanations of discrepancies repeatedly encountered while trying to account for the results of experimental proton shielding tensor measurements by the Multiple Pulse Selective Averaging methods in Solid State NMR. This work, particularly on the single-crystal of pyromellitic acid di-anhydride, opened up (as was pointed out in the discussions of the published paper *S. Aravamudhan, U.Haeberlen, H.Irngartinger & C. Krieger, Mol. Phys. Vol. 38, P 241, Year 1979*) a two pronged investigation of the consequences: 1) To study the possibilities of calculating INTRA (in exclusion of the INTER) molecular contribution to the shielding tensors as arising due to the induced fields by simple point dipole contributions. (Such a calculation would require appropriate sets of Susceptibility tensor values which in the paper above were obtained from Flygare's data - [Click & Jump](#) to remark below - and such choices of empirical data for calculation of other physical quantities would be beset with ambiguities as also pointed out at the "discussion" of the publication by Aravamudhan et al.) And, 2) to find methods of extending the considerations of intermolecular calculations, to the total macroscopic extent of the specimen; instead, of the only semi-microscopic (of about 100 Angstroms extent) elements. These should enable the simple basis of dipole contributions to be understood more comprehensively from the intra- to intermolecular consequences without the accompanying obscurities due to the involved mathematical procedures, which render all the explanations to be beset with a kind of abstractness, which causes discomfitures while applying in Chemical contexts. On the aspect (1) a poster presentation could result at the Joint ISMAR-CA'98 held at the Technische Hochschule Berlin in 1998. The aspect (2) above is the matter dealt with in the presentation at the **2nd Alpine Conference on Solid State NMR, Chamonix Mont-Blanc, France during 9-13 Sept.2001.**

These aspects have been presented (in steps), at the annual **Symposia of the National Magnetic Resonance Society, INDIA.** Hence, the present achievement is founded firmly on the results of the work as Post Doctoral Fellow during 1975-77, and the information gathered by literature survey while being at the NCL, Pune. In addition, further supplementary assistance was available from CSIR labs, to get copies of the published reference materials. The earlier efforts to realize were all in the form of several M.Sc., Project Works (each of only six months duration) at the NEHU, Chemistry. A great deal remains to be inferred by intensive efforts, and communicate them as publications in Journals. The possible applications of these simple calculation procedures have been pointed out broadly in the poster presentation at the **XIII International Biophysics Congress in held in New Delhi in September 1999 and this participation was supported by an INSA grant.** The research results, which are contained in the presentations, are all the outcome of the work carried out during the tenure of appointment as teacher in the Department of Chemistry, North Eastern Hill University, Shillong. The results are being further pursued with the purpose of finalizing them for publication in refereed Journals. Most of the efforts had been resulting only in single author presentations. The publication includes an earlier Presentation in XIII International Biophysics Congress and related Biophysical & Biochemical meetings.1]. The copy of the ABSTRACT uploaded & submitted at the Web abstract-Submission box/page of the XIV I.B.C. is being included in these pages. A grant could forth come from the organizers of the second Alpine Conference on SSNMR for the participation.

S.Aravamudhan

Author of the Contribution to XIV I.B.C., Buenos Aires, Argentina, 2002

Lecturer, Department of Chemistry, North Eastern Hill University, Shillong, Meghalaya.

HR PMR Experimental Results on Single Crystals of PMDA, by multiple-pulse, line-narrowing technique: determination of full shielding tensor of Protons (**1977-'78**) . Attention is drawn here to the necessity of having to make spheres of single crystal specimen for such measurements (hence difficult experiment). See (next sheet) the possible protocol of procedure that now appears viable for measurements on arbitrary shapes of single crystal specimen.

The clarification obtained on the way the Inter-molecular and Intra-molecular Shielding Contributions can be disentangled. (**1978-'79**)

Such separation of contributions of induced fields (*proportional to shielding parameters*) into its components, results in further clarification (**1979-and later**) on the role (*considerations from before 1975*) of macroscopic bulk susceptibility (*condensed matter - a possibility for quantitative demarcation of Lorentz Sphere (IJP., Vol.79(9), p 985-989 (2005)), / magnetic materials*) and the molecular susceptibilities (*the bond and atom susceptibilities*).

The considerations of inter-molecular shielding as a semi-micro aspect, requires the consideration of the bulk macroscopic shape dependences on the one hand, and the micro / molecular susceptibilities for the possibility and necessity to fragment the molecular susceptibility, on the other. This led to the formulation of two aspects (**1980 onwards**):

2) It became necessary to look for possibilities of improving the validity of Point-dipole approximation. This should enable the applicability for smaller sizes of regions of charge circulations, and at shorter distances for molecular dimensions.

1) It became necessary to look for possibilities of simplifying the evaluation of integral forms arising while handling the bulk, macroscopic specimen shape dependences of induced field contributions.

Both aspects as above seemed to get a solution (**1990 onwards**), in view by the alternate Summation Procedure (**1980-1990**) for calculating induced fields within materials and molecules. And it seemed to provide a way to circumvent the impediments by providing elegant and simple method to handle magnetized materials comprehensively (from the molecules to the bulk materials (**NMRS1999** presentation) and even find methods, hitherto unknown, to handle cases arising in Biological contexts. Thus, the concept of point dipoles seem to stand validated even more as a reality than simply a mathematical simplicity and consequence of such methods. The role of susceptibility and circulating charge densities, in inducing dipole moments, is tenable for further investigations by calculations of induced field distributions. Comparing the results from quantum chemical calculations of shielding & susceptibilities (**Magnetic dipole model for intra molecular shielding-ISMAR/CA1998**) and in turn, accounting for induced field distributions by calculation using magnetic dipole model, and by experimental determination of shielding and susceptibilities. Abstract submitted to ISMAR2013 conference included on page-6-

[Envisaging a Protocol of Procedure \(download from webpage\)](http://sravamudhan.tripod.com/csir_schm_sa/id24.html)

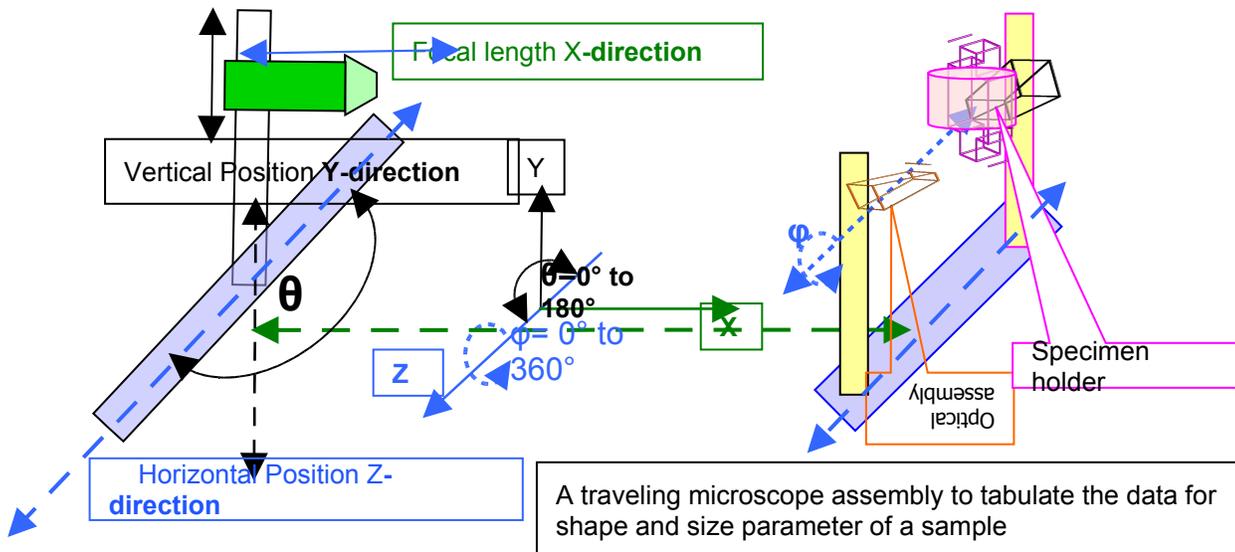
http://sravamudhan.tripod.com/csir_schm_sa/id24.html

http://saravamudhan.tripod.com/sitebuildercontent/sitebuilderfiles/es_3_draft_project_proposal_m.pdf

1. Define ϕ to be equal to zero, for the disposition of ZX plane above.
2. Every setting along the vertical Y-axis would define the parallel set of [1 N_y 1 / 'ZX'] planes, every setting along the y-axis at equal intervals (convenient & arbitrary) counted sequentially by serial index N_y = 0,1,2,3,4.... and this sampling is made as much smaller an interval value as possible.
3. At each 'N_y' value (corresponding to that assigned y coordinate) sampling along the X-axis, at equal intervals serially from left to right with index N_x = 0,1,2,3,4... would result in recording at specified X-coordinates, and from the focal length for the give setting of x,y would result in the z-coordinate.
4. Thus a table of x,y,z can be constructed for $\phi = 0$
5. These are (x,y,z) values with origin(0,0,0) located outside the specimen, and a transformation, shifting of origin can be effected to get these set of values (x,y,z) with respect to an origin located inside the specimen.
6. With respect to the internal location of the origin, and using the same disposition for the coordinate axes directions, the following identities can be used to get a set of polar coordinates.
 $x = r \cdot \sin(\theta) \cdot \cos(\phi)$; $y = r \cdot \sin(\theta) \cdot \sin(\phi)$; $z = r \cdot \cos(\theta)$
7. The measurements can be similarly made for other values of ' ϕ '. Depending on how regular (non-ellipsoidal) shape and what symmetries are conspicuous for the shape, the values of ' ϕ ' can be chosen. For example in certain shapes, a measurement for $\phi = 0^\circ, 90^\circ$ would suffice to describe the macroscopic shape in terms of the set of r, θ , ϕ values.
8. Then the 'complete' set of θ , ϕ values thus measured at experimentally convenient mesh of sampling may have to be subjected to a smoothening appropriately, define 'complete' set of values to be able to describe the close packing criterion for calculation by the summation procedure.

What are the optimum orientations? ; And, how many samples are required to get the morphological details without losing information on the shape factors is a matter of concern similar to the Concerns in the article in Advances in Magnetic Resonance, Vol. (?), Academic Press, year? by **John A Weil** (Reference No.7 (?) listed in "Pyromellitic Acid.....Proton Shielding", S.Aravamudhan, U.Haeberlen, H.Irngarter and C.Krieger, Molecular Physics, 38, 241 (1979)

The above is intended to take into account comprehensively the (continuum) bulk susceptibility contributions at given proton site, which along with the (discrete) intermolecular near neighbor contributions gets added on to the **INTRA MOLECULAR** shielding tensor, while obtaining the Proton Shielding Tensor parameters by a measurement on Single Crystal specimen by the Multiple Pulse Line Narrowing Technique.



Abstract submitted to ISMAR2013 & accepted for Presentation.

<http://www.ugc-inno-nehu.com/events-2013.html#ISMAR2013>

Calculating Intra-molecular Proton Shielding Tensors Using Magnetic Dipole model; Possible Procedures and Prerequisites

S.Aravamudhan

Department of Chemistry, North Eastern Hill University,
Shillong 793022 Meghalaya; INDIA

The necessity for trying to calculate the intra molecular proton shielding tensor has been enumerated in the introduction by this author (1). A feasibility study has been reported (2) at the ISMAR-CA'98. Those results indicated that it seemed possible to obtain results which can be compared with experimental values for the case of the peripheral proton in the benzene ring, However, at that time, no comparison with QM calculations were made though the comparison with experimental results on aromatic protons was reported. Moreover, the contribution of the C-H bond susceptibility to the proton bonded to that carbon could not be used for reasons of reasonable validity of the point dipole approximation. The effort to apply the magnetic dipole model for the calculation of demagnetization factors (3) proved that depending on the parameters used for fragmenting a susceptibility tensor, the point dipole approximation could become valid better even at much closer proximity to the proton location (4). Thus, the possibility of using this model for details could be envisaged typically for the case of benzene molecule (5). In the present contribution, the results obtained earlier (2) could be improved, and a comparison of the results of the use magnetic dipole model could be compared also with the QM calculations of Shielding Tensors. In addition as envisaged in (4) and (5) the C-H bond contribution to the shielding of the attached proton could also be added for inclusion instead of trying to use a value derived from QM calculations on ethylene proton. These results would be discussed in view of the necessary further improvements. Such efforts might eventually provide an explanation to the remark made earlier (6) about the atom and bond susceptibility tensors obtained from the very same set of Molecular Susceptibility values.

- (1) <http://saravamudhan.tripod.com/index.html>
- (2) <http://saravamudhan.tripod.com/id2.html>
- (3) <http://saravamudhan.tripod.com/id4.html> <http://saravamudhan.tripod.com/id5.html>
<http://www.ugc-inno-nehu.com/isc2009nehu.html>
- (4) <http://saravamudhan.tripod.com/id6.html> http://nehuacin.tripod.com/pre_euomar_compilation/id5.html
<http://nehuacin.tripod.com/id6.html>
- (5) <http://saravamudhan.tripod.com/id3.html>
- (6) On page 682, at the end of first column by W.H.Flygare, Chemical Reviews, Vol.74, page 653 (1974).

http://aravamudhan-s.ucoz.com/poster_sheets_ampere_lille.html

The following article copy / pdf file is linked at the above URL;

Note the **download link** below

Magnetic Susceptibility: Further Insights into Macroscopic and Microscopic Fields and the Sphere of Lorentz

C.J. DURRANT,¹ M.P. HERTZBERG,¹ P.W. KUCHEL,²

¹ School of Mathematics and Statistics, University of Sydney, New South Wales 2006, Australia

² School of Molecular and Microbial Biosciences, University of Sydney, New South Wales 2006, Australia

Correspondence to: P.W. Kuchel; E-mail: p.kuchel@mmb.usyd.edu.au

Concepts in Magnetic Resonance Part A, Vol. 18A(1) 72–95 (2003)

(Download Article link: http://aravamudhan-s.ucoz.com/geo_export/0/suscetibility.pdf)

CONCLUSIONS as on page 91-92 of this article

“In conclusion, we can finally consider the validity of the assumption of spherical symmetry for a molecule averaged over all its orientations:”

Hence, we have shown that, the mathematical constructs presented above are well defined and allow the bulk susceptibility shift to be calculated on a more rigorous basis than hitherto. In practice, an NMR experiment samples a large number of nuclei in a macroscopic volume over a macroscopic time interval, and each will experience a fluctuating environment as the neighboring molecules move around. As a result, the molecules will not experience a single average field but a spread of field strengths. This fluctuation will appear as a broadening of the resonance line about the mean value that can be calculated as described here. In principle, the size of the fluctuations can be estimated from the width at half height of the NMR spectral line if the geometric factors are known accurately.

(see previous accompanying article).----→ refers to the publication in Concepts in magnetic resonance



Remark by Dr. S. Aravamudhan, in view of the studies on induced field distribution & NMR chemical shifts:

As in the publication cited above, the necessity to seek an averaged orientation for a required molecular spherical symmetry is a microscopic molecular level effort to obtain simplified approaches as for the constraint to only regular ellipsoidal shapes for the case of macroscopic specimen. Hence, calculations of induced fields are intricately linked with the corresponding shapes over which the distributions are required. And, either by methods formulated with complicated integrals or a simple summation of elementary contributions all stem from the induced point dipoles expressed as susceptibility induced magnetic moments or elementary (infinitely small) current loops inducing fields which is distributed over extent of the relevant region. Thus when it becomes possible to derive equations with parameters, which can be altered independent of the actual “size” of the region, then it makes possible to apply the point dipole approximation at small distances, which effectively improves the validity of point dipole approximation. With such a facility, it seems to become simply a matter of addition of finite small quantities, instead of the infinitely small elements, which require the setting up of integrals to evaluate the sum.

Key words/phrases:

Material Bulk Susceptibility ; Molecular Susceptibility ; induced moments; induced fields ; demagnetization factors ; specimen shape dependences ; Molecular Fragments ; Functional Groups ; Susceptibility of Molecular Fragments ; Susceptibility and Shielding-NMR chemical shifts ; susceptibility values from measured shielding; Quantum Chemical Calculation of Susceptibility and shielding and the Consistency of the Quantities calculated and measured. Shielding as induced secondary field; induced field distributions due to susceptibility; Magnetic dipole model; Point Dipole Approximation (PDA) ; Validity Criteria for PDA

From the concluding section of the Draft manuscript of [Dr.S.Aravamudhan](http://nehuacin.tripod.com/id1.html): **for the MRS Fall 2006** <http://nehuacin.tripod.com/id1.html>

This is all in static field distributions in solids, the case of I.V.E. in the liquid state is much less tractable since the time, and space averages have to be considered. If this recent method of treating the continuum bulk contribution is extended to liquid state and by subtracting its effect from the experimental value, it would be possible to ascertain the contribution of I.V.E (discreteness is out of the purview in liquids) can be estimated. Since this summation method simplifies handling non-regular shapes, it might be providing more insights into the IVE contributions in liquids.



TEXT BELOW for an outlook:

The *last section (page-10)* of the research proposal of [Dr. S. Aravamudhan](#);

The proposal has been drafted in accordance with the Formats prescribed for applying to CSIR / “Emeritus Scientists” scheme.

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. The discreteness of the contribution from adjacent sites [to result 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_euromar_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 Investigator 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