21st International Conference on Magnetic Resonance in Biological Systems (ICMRBS) Hyderabad, India (January 16-21, 2005)

60th Anniversary of the Discovery of Nuclear Magnetic Resonance

October 6, 2005

To Whom It May Concern

This is to Certify that Dr.S.Aravamudhan, Department of Chemistry, North Eastern Hill University, Shillong, participated in the XXI International Conference on Magnetic Resonance in Biological Systems ICMRBS2005 held during 16-21, January 2005 in Hyderabad and was present at the venue to make the poster presentation on the Abstract material entitled: "*Disentangling the Bulk Susceptibility Medium-Effects from the Molecular Local Chemical Shift Changes in Heterogeneous Biological Systems*" which he had submitted on time, and which was reviewed by a Scientific Committee and adjudged for poster presentation.

K.V.R.Chary

Intrduction

DISENTANGLING THE BULK SUSCEPTIBILITY MEDIUM-EFFECTS FROM THE MOLECULAR LOCAL CHEMICAL SHIFT CHANGES IN HETEROGENEOUS BIOLOGICAL SYSTEMS:

INTRODUCTION:

Most often when NMR Chemical shifts are measured experimentally, the bulk susceptibility effects do not play dominating role in determining the induced field values at the specified nuclear sites. But, there are instances when the contribution to the induced fields at the Proton (Nuclear site) can be large compared to the specific molecular contributions, which is the factor that causes chemical shift differences. Due to the bulk Susceptibility or due to the molecular susceptibility or, more particularly, due to the Group, Bond or Atom susceptibilities within the molecules, the contribution to the induced field is basically attributable to corresponding changes in the appropriate electron charge circulation. Hence it becomes necessary to know the various electronic structural changes and the differences in their dependences on variations in the experimental conditions. But these information **cannot be taken for granted as already known** because in the Biological Systems the **study of the variations in Chemical Shifts is intended precisely for the purposes of deriving these information.**

Hence efforts are made to obtain standardized information correlating the various experimental conditions and for each type of susceptibility, what are the trends for the induced field contributions and their variations. The intra molecular situations are reasonably well characterized and documented but if the bulk susceptibility contributions dominate, the molecular differences, being much smaller in magnitude, may not be observable with any significance. But, The mechanism for the induced field contributions in the context of NMR is so basic for the utility of NMR technique, it is still possible to keep on trying to disentangle the bulk susceptibility contributions from chemical shift differences making the NMR technique and its application to Biological Systems as Frontier efforts to make progress on the information retrieval from the biological processes.

To really appreciate that progress can be made, it becomes necessary, time and again to recapitulate what is already studied and known, because retaining the comprehension while trying to spring out from the edge of broad platform of the vast documented information.

Recently certain progress[1] could be made on the Demagnetization factor Calculations by evolving a simple summation procedure for calculating the induced field contributions within the magnetized materials. This is a question of making available a simple mathematical procedure for a context wherein the arguments for **"macroscopic averaging and microscopic averaging within the magnetic materials"** compound each other while trying to know the actual field at a point within the sample, which acquires a magnetization due to the presence of an external magnetic field.

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[1] Contribution by **S.Aravamudhan** at 3rd Alpine Conference on SSNMR, New Concept and Applications http://geocities.com/amudhan_nehu/graphpresent.html and at the 17th EENC and 32nd Ampere http://geocities.com/saravamudhan1944/eenc_ampere_lille.html

Continuation……… **Introduction &Index to Poster Sheets**

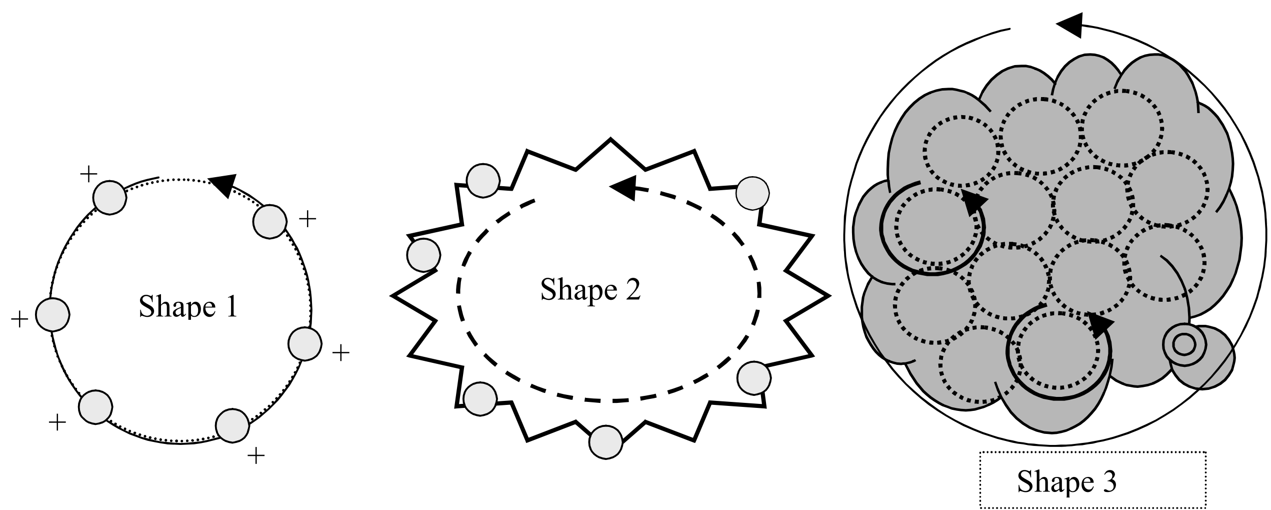
It is intended here to display a few pages pertaining to the basic aspects which govern the definitions and laws governing the induced fields which are inherent in the interpretation of chemical shift information along with a generalized account of the induced fields arising due to Bulk Susceptibility of the material and due to the induced magnetic dipole moments within the sample. These considerations are extended to include a description of a simple summation procedure for calculating induced fields due to the bulk susceptibility of the medium. Then, a discussion of the advantages of this mathematical procedure is given for the context of the experimental situations pertaining to biological systems, all stated in terms of the characteristics of the characteristics of the magnetized samples and how these contexts can become tractable by this simpler procedure. Particularly the magnetic point-dipole approximations, which become a very convenient way to visualize and calculate induced field contributions is discussed with the perspective of how to make this approximation valid even I the contexts which has hitherto been considered as situations where such simple magnetic dipole models would fail. Thus hypothetically the situations encountered in biological systems are dealt with and no detailed effort is intended in the following poster sheets, to present any application to biological systems. However, it is the application to actual biological systems which is the long term perspective of this presentation which is possible because of the progress made in the context of interpreting HR PMR spectra in single crystalline solids.

INDEX:

Charge Cloud Descriptions, Circulatory Movement of Charges, The CURRENT FLOW

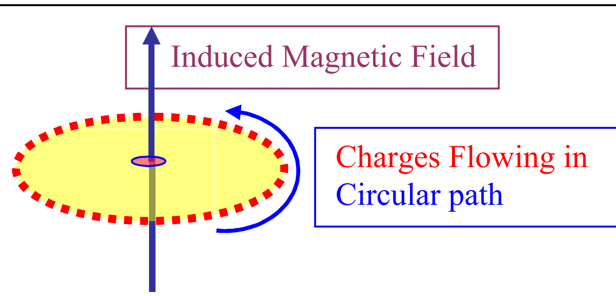
While explaining the presence of a **"dipole moment"** by considering the poles which, depending on the context, the poles may be the "electrical (positive and negative) charges" or the ["magnetic charges"] magnetic "north" and "south" poles. In either case a dipole moment can be defined: in the former case it would be *electrical dipole moment* and in the latter case it would be *magnetic dipole moment*

In the case of flowing electrical charges, the current thus flowing can cause a magnetic field, which can be associated with the flow characteristics and the amount of the electrical charges. The magnetic field thus arising can be calculated and the direction of the field determined. This can be the attribute "dipole moment" for the flowing charge systems.



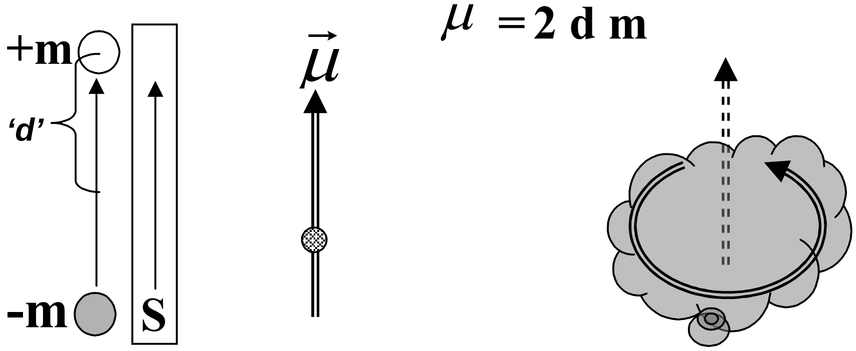
Flowing positive charges

In each of the above cases a magnetic moment can be attributed for the charge flow. In the case of SHAPE 3 the charge cloud is depicted. The total charge cloud can be considered as small, charged, volume elements inside the charge cloud. These volume elements each can be attributed a small dipole moment and the total dipole moment associated with currents in the charge cloud can be obtained by a vector addition of the individual elemental dipole moments.



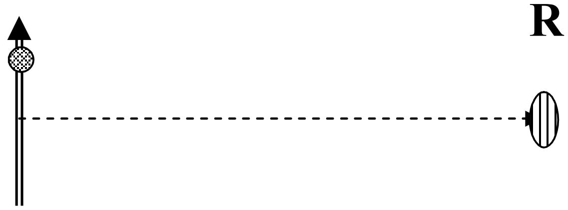
Charge circulation, Magnetic Moment and the point dipole approximation

$\vec{\mu} = 2\ d\ m$



The approximated radius of this charge cloud has to be taken into account while deriving the "distance" factor **d**

In case of either the electrical or the magnetic dipole moments a simple arrow can serve the purpose to indicate the presence of a "Dipole" as located at a given point



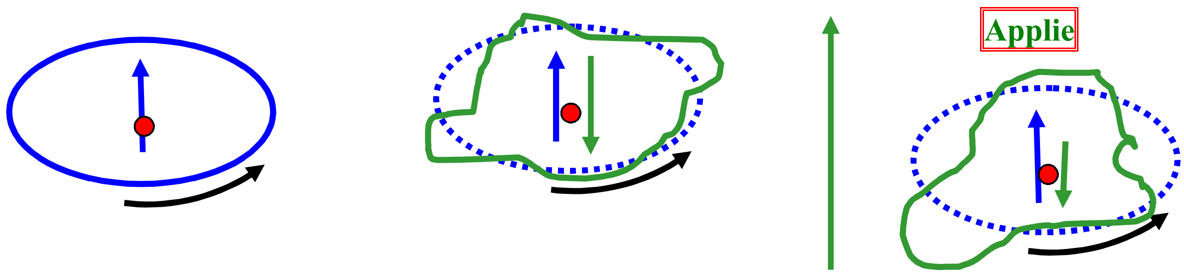
While considering the Field due to the dipole moment at 'R' it is possible to consider the two poles separately and find the contribution from each pole and sum up to get the total.

Instead of each time considering the poles of dipoles separately , it is possible to get an equation for this total at R by a single equation using the dipole moment. This implies that the distance **d** has to be considered while calculating the field at a distance **R.** It turns out that if **d** ≅ **R** then, the calculations result in unrealistic values. For reasonable application the value of **R >> d.** This means **R** ≥ **10•d.** This is referred to as the POINT-DIPOLE approxomation. It is a consideration as to at what values of the distance **R** the given dipole can be arising from a single point and not from the consideration of the length **d** characteristic for the value of the moment **|μ|.**

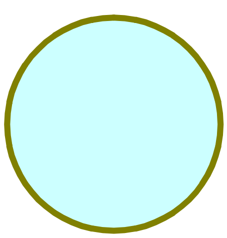
At the point 2 "outside the cloud where the 'radius' would be small compared to distance 'R' to the point The point dipole approximation is more valid than at 1 "within' the cloud itself. In fact such an approach to aplly POINT dipole approximation at 1 would be not at all justifiable.

Induced Fields due to circulation of Electrons Causing Shielding, Demagnetization effects

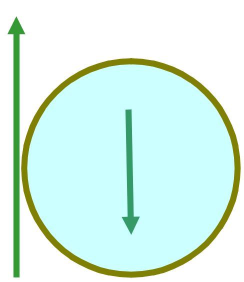
In Atoms and Molecules the electrons are in constant revolution in Orbitals which should be constituting a constantly flowing currents . These flowing currents should be inducing magnetic fields at the center where the nuclei are located in atoms,for example. Thus at the nuclear site there would be induced magnetic fields whether there is an externally applied magnetic fields or not. Applying the external ,large,steady fields alters the way the electrons were flowing in the system before the application field and it is these changes in induced fileds which are manifest while measuring the Shielding effects as the Chemical Shift parameter. The alteration of the flow of electrons could be either a change in the velocity of electrons or the shapes of the orbitals.



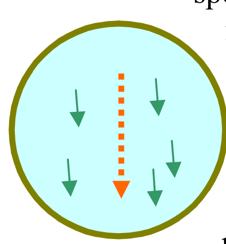
Alterations of shape of orbitals *can come about because they are bonded in molecules i.e., in different bonding situations. Thus for the same applied field strength, the* **changes in the induced fields in presence of external field** ***can be different. According to Lenz's Law these induced fields have directions opposite to the direction in which the Magnetic field is applied. Paramagnetic and diamagnetic chemical shift contributions must be related to the sense in which circulations are altered relatively and whether changes can be accounted for by the deviations from spherical symmetries***.



Macroscopic specimen



Macroscopic Diamagnetic Specimen Magnetized in Magnetic Field



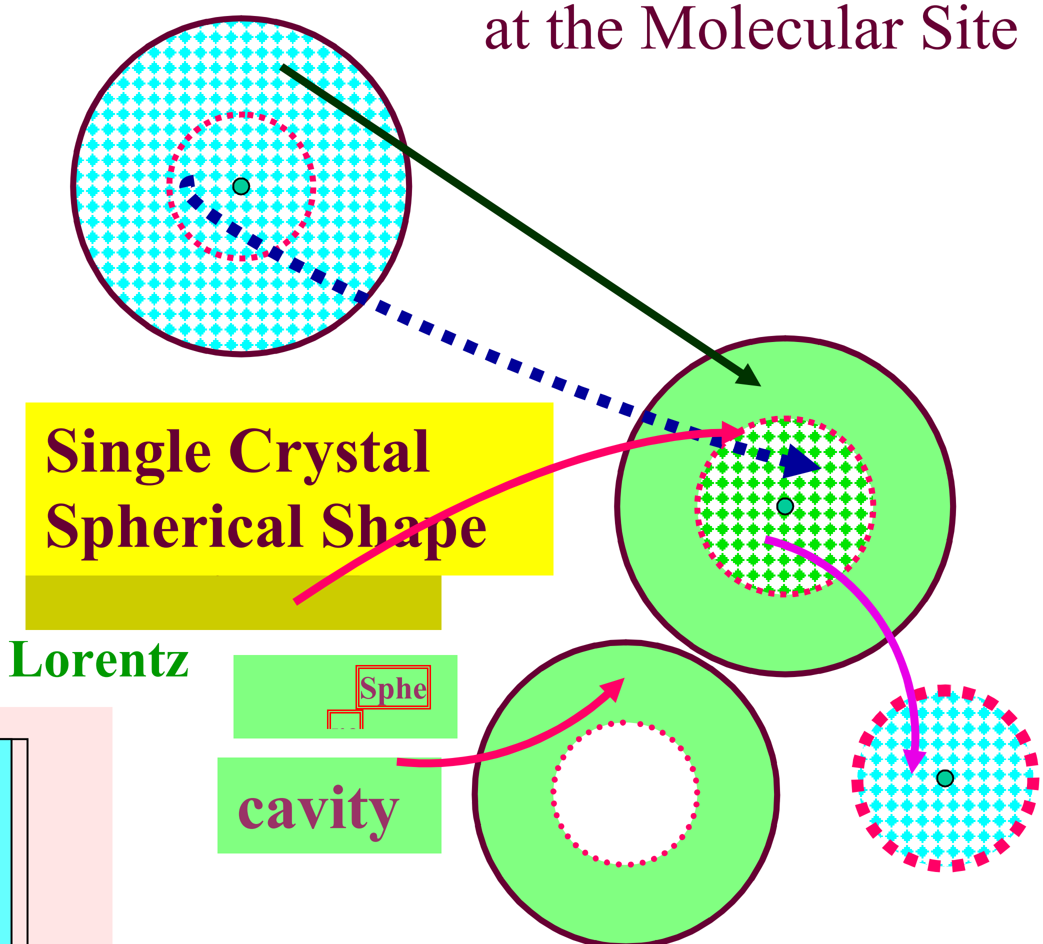
The induced magnetic moment represented at the center of the specimen is due to its inherent magnetic susceptibility. Whether the magnetic moment induced should be at the center of the specimen or not cannot be answered in any simple way. The single moment at the center can be ***hypothetically*** subdivided into several small components and distributed into several locations within the specimen the total adding upto the same value. Then the net induced fields due to these small moment be the same as that of the total placed at center? If not, should an interaction between these subdivided moments be considered which would be absent if only the single total was considered?

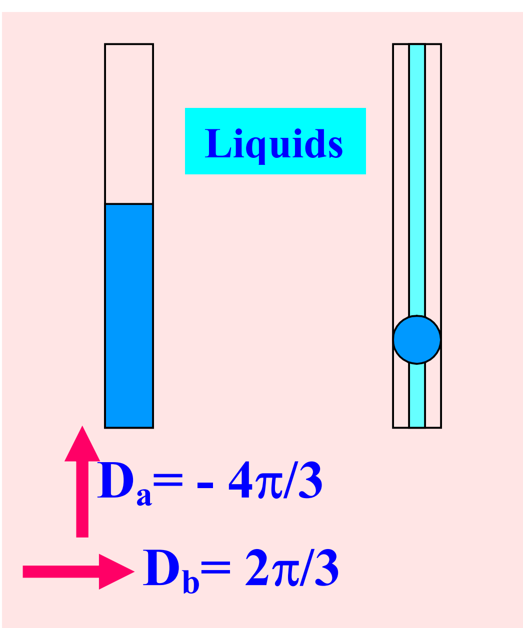
A Recapitulation

SOLIDS

Induced Fields at the Molecular Site

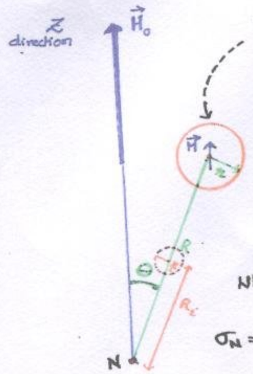
For HR PMR measurements the requirement to have the single crystal specimen in the spherically shaped outer-form had been stringent.
This requirement had been implemented because of the well known, **Spherical Cavity** in which the induced fields can be made zero for such an outer spherical shape





The use of spherical sample 'tubes' for HR PMR measurements in Liquids to reduce the Bulk

DMSBSB – "*APPLICABILITY*……………. *STRUCTURE DETERMINATIONS*" - **S.ARAVAMUDHAN** **Sheet # 3.**



SPHERICAL SAMPLE WITH A HOMOGENEOUS, ISOTROPIC VOLUME SUSCEPTIBILITY χ_v per unit volume, radius r

Magnetization $\vec{M} = \chi_v \cdot v_{sphere} \cdot \vec{H}_0$

$\|M\| = \chi_v \frac{4}{3}\pi r^3 \|H_0\|$

This magnetic moment M induces a field at N $= \sigma_N \|H_0\|$

When $R \gg r$

$$\sigma_N = \chi_v \frac{4}{3}\pi r^3 \frac{(1-3\cos^2\theta)}{R^3}$$

$$\sigma_N = \chi_v \frac{4}{3}\pi \frac{1-3\cos^2\theta}{R^3} \cdot r^3$$

$$= \chi_v \frac{4}{3}\pi \left(\frac{r}{R}\right)^3 1-3\cos^2\theta$$

For another sphere with r_i and R_i such that $\frac{r_i}{R_i} = \frac{r}{R}$

$$\sigma_N' = \sigma_N$$

d_i : 0.0109027 mm

r_i : 0.0054513 mm

$\frac{R_i}{r_i} = 45.8602$

Hence $R_i \gg r_i$

$\chi_v = -2.858 \times 10^{-7}$

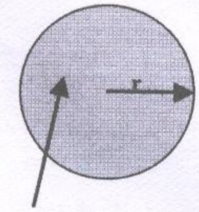
for $\theta = 0°$ $\sigma_N' = +0.239278 \times 10^{-10}$ $\approx 2.4 \times 10^{-11}$

$= \sigma_N$

Sheet 4

Radius of sphere = r

Volume of sphere= $V_{sph} = 4/3\,\pi\, r^3$



$\chi_{sph} = V_{sph} \cdot \chi_v$

Magnetized Sphere

Uniform Volume Susceptibility χ_v

for each θ and each dipole

$$\sigma_\theta = \chi_{sph} \frac{(1-3\cos^2\theta)}{R^3}$$

$$= \chi_v \cdot V_{sph} \cdot \frac{(1-3\cos^2\theta)}{R^3}$$

$$= \chi_v \cdot 4/3 \cdot \pi\, r^3 \frac{(1-3\cos^2\theta)}{R^3}$$

$$= \chi_v \cdot 4/3 \cdot \pi \cdot \frac{r^3}{R^3} \cdot (1-3\cos^2\theta)$$

i.e., $\sigma_\theta^i = \chi_v \cdot 4/3 \cdot \pi \cdot \frac{r_i^3}{R_i^3} \cdot (1-3\cos^2\theta)$

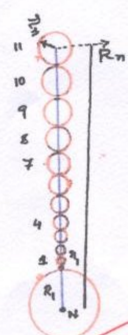
↖ Constant $= R_c$.

Sheet 4

An explanation for the factor R_i / r_i = **45.8602** appears on **Sheets 6 & 11**

Equation for the number of dipoles '**n**' Stacked/ close-packed along a vector length is given ⟹

$\sigma^{total} = \Sigma^n{}_i\, \sigma^i$ explained further on **Sheet 6**



Given R_1 and R_n and Ratio constant $\frac{R_i}{r_i} = R_c = 45.86$

number of closely packed spherical dipoles

$$n = 1 + \frac{\log(R_N/R_1)}{\log\left\{\frac{R_c+1}{R_c-1}\right\}}$$

$$n = 1 + \frac{\log(R_N/R_1)}{\log\left(\frac{46.86}{44.86}\right)}$$

obtaining $n = 1 + \frac{\log R_N/R_1}{\log\left\{\frac{R_c+1}{R_c-1}\right\}}$ this equation was an important step.

for $\theta = 0$, for 1 dipole $\sigma_N = 2.4 \times 10^{-11}$

Hence $\sigma_N^{(total)} = \sum_n \sigma_N$

$= n \times 2.4 \times 10^{-11}$

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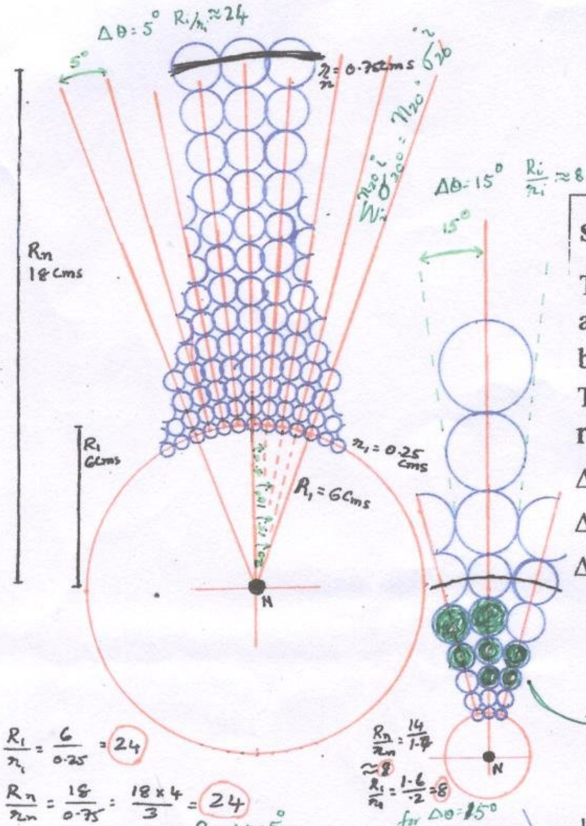
DMSBSB – "APPLICABILITY……………. STRUCTURE DETERMINATIONS" - S.ARAVAMUDHAN Sheet # 4.



Sheet 5

The situation of close-packing of spheres along a radial vectors with the angle Δθ between them being 5° is illustrated.
This situation with $\Delta\theta = 2.5^\circ$ results in the ratio R_i / r_i value 45.8602

$\Delta\theta = 15^\circ \quad R_i / r_i \approx 8$

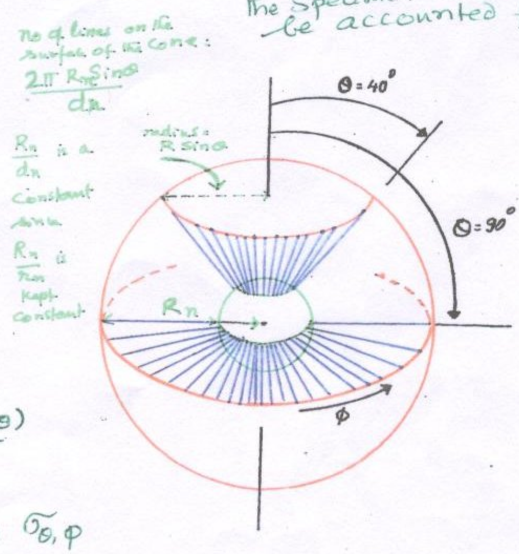
$\Delta\theta = 5^\circ \quad R_i / r_i \approx 24$

$\Delta\theta = 2.5^\circ \quad R_i / r_i \approx 48$
$= 45.8602$ as in Sheets 6&11

When the Volume elements are spherical & close packed there still remains voids. The magnetized material corresponding to this void would not be considered for the Induced Field contribution and hence the contribution of all the material of the Specimen would not be accounted for

Sheet 5

If the site where the Induced Field is calculated is represented by 'N' and if the point N located at the centre of the macroscopic specimen (for all these calculations a microscopic cavity around the point 'N' hypothetically considered irrespective of where the point 'N' is located within the macroscopic sphere) the dependences on **r,θ & φ** are as follows: number of dipoles packed '**n**' depends on the length **r.** i.e., $\mathbf{n_\theta}$ for a given value of Δθ=2.5/5/15/...

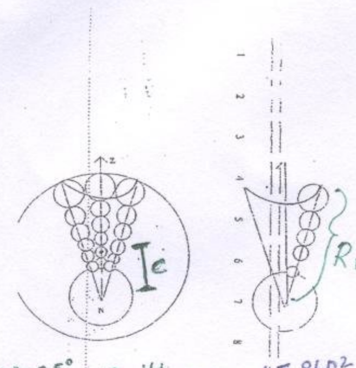


n_θ depends on $|\vec{r}| = r$ only $= R_n$ along $\vec{R_n}$ for given θ

each dipole $\sigma_\theta = \chi_{sph} \cdot \frac{(1-3\cos^2\theta)}{R^3}$

$$\sigma_\theta = \sum_i^{n_\theta} \sigma_\theta^i = n_\theta \cdot \sigma_\theta^i$$

$$\sigma_{\theta,\varphi} = \sum_i^{n_\theta} \sigma_\theta^i \cdot n_\theta \cdot 2\pi \frac{R_n}{d_n} \cdot \sin\theta = \sigma_{\theta,\varphi}$$



$\Delta\theta = 2.5°$

no of lines $= \frac{360}{2.5} = 144$ $\quad R_i/r_i = 45.8602$

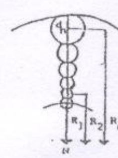
$R_n/d_n = 22.93$

$d_1 = 2\pi R_1/144$

$R_n = -c\cos\theta + \sqrt{R^2 - c^2\sin^2\theta}$

$n = 1 + \frac{R_n/R_1}{.01894}$

figure III.



$r_n = \frac{d_n}{2}$, n = number of spheres

$r_n = \frac{d_n}{2}$

n = number of spheres

FIG III: Variation of radius of the sphere as the distance from the centre varies, and, Identification of distances R_i and diameters d_i for calculation of n.

$\sigma = \sigma_i = \chi_v \cdot \frac{4}{3}\pi r_i^3 \cdot (1 - 3\cos^2\theta)/R_i^3$

$\frac{r_n}{R_n} = r_i/R_i$: constant, closely pack to line-up along the direction 'θ' from magnetic field

$\sigma_1 + \sigma_2 + \ldots \sigma_i + \ldots + \sigma_n = n.\sigma$

$\sum^n \sigma_i = n.\sigma$

$\sum \sigma^i = \sigma^1 + \sigma^2 + \sigma^3 + \ldots + \sigma^n$

$\sigma_\theta^i = \chi_v \cdot 4/3 \cdot \pi \cdot r_i^3/R_i^3 \cdot (1 - 3\cos^2\theta)$

$= \chi_v \cdot 4/3 \cdot \pi \cdot (1 - 3\cos^2\theta) \left\{ \frac{r_1^3}{R_1^3} + \frac{r_2^3}{R_2^3} + \ldots + \frac{r_n^3}{R_n^3} \right\}$

$\sigma_\theta = n_\theta \sum_i^{n_\theta} \sigma_\theta^i \quad = \quad \frac{r_1^3}{R_1^3} = \frac{r_2^3}{R_2^3} = \ldots = \frac{r_n^3}{R_n^3} = R_c^3$ constant

If the nucleus N is at the centre of Macroscopic Sample, then for all θ (the polar angle)

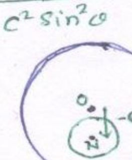
$R_n = R_n^{\theta_1} = R_n^{\theta_2} = R_n^{\theta_3} = R$ = the radius of Mac sphere

Hence calculation of R_n is to simply replace R_n by R for all θ values.

If N is not at centre, i.e., the $|\vec{c}| \neq 0$ then

$R_n^\theta = -c.\cos\theta + \sqrt{R^2 - c^2\sin^2\theta}$

$n^\theta = 1 + \frac{\log(R_N^\theta/R_i^\theta)}{\log\left(\frac{R_c + 1}{R_c - 1}\right)}$



IS OFF CENTRE N

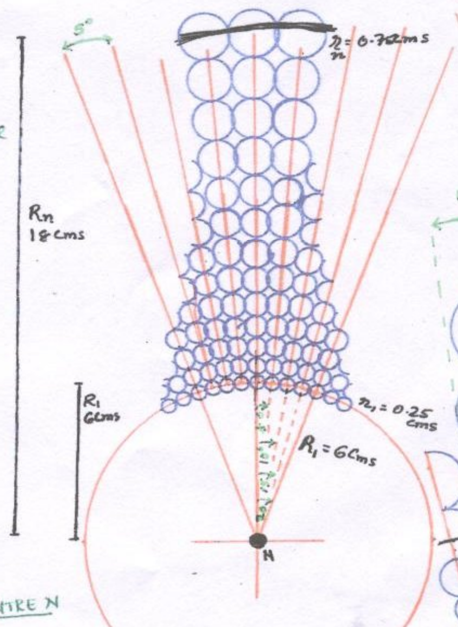
$n^{\theta_1} \neq n^{\theta_2} \neq n^{\theta_3} \ldots$

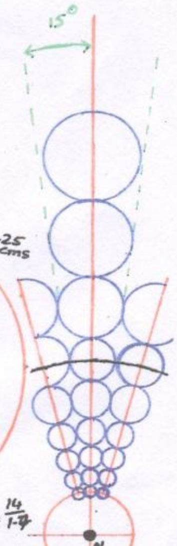
$n_{\theta_1} \neq n_{\theta_2} \neq n_{\theta_3} \ldots \neq n_{\theta n}$

for $|\vec{c}| \neq 0$

$n_{\theta_1} = n_{\theta_2} = n_{\theta_3} \ldots = n_{\theta n} = n$

Since $R_n^\theta = R$





$\frac{R_1}{r_1} = \frac{6}{0.25} = 24$

$\frac{R_n}{r_n} = \frac{18}{0.75} = \frac{18 \times 4}{3} = 24$

$\frac{R_n}{r_n} = \frac{14}{1.4} \approx 8$

$\frac{R_1}{r_1} = \frac{1.6}{.2} = 8$

TABLE II

Sl. No.	R (mm)	R_1=r (mm)	C (mm)	σ_+ (ppm)	σ_- (ppm)	$\sigma = \sigma_+ + \sigma_-$ (ppm)
1	2.5	0.5	0	1.1535449	-1.1527074	0.0008375
2	2.5	0.25	-0.25	1.633834	-1.6329986	0.0008354
3	2.5	0.25	-2.25	1.0577755	-1.0570753	0.9007002347
4	2.5	1.0	0	0.67140974	-0.67091247	0.00049727

Thus the results of the present work show that the cavity field induced within a homogeneously magnetized spherical sample is equal to zero even when the centres of the inner sphere and outer sphere do not coincide (cases 2 and 3 in Table II). This result is known and thus the calculations based on magnetic dipole model reproduce the known results.

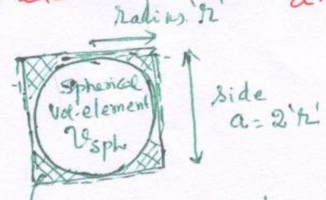
From Computer Program −0.000598

For field along x-axis 0.000988

In a homogeneously magnetized material which has a macroscopic spherical shape the cavity inside can be placed at any point in the medium and at every one of such points the calculated induced field must be zero. Illustration in diagram below and values in Table II on the left side

Every one of the Spherical close-packed volume elements must be surrounded by a Cubical element to make use of the whole material and not to leave out voids in the medium taken into account

ELLIPSODS are considered in Sheet 7.



a Cube within which the Spherical volume fits in

$\therefore v_{sph} = 4/3 \pi r^3$

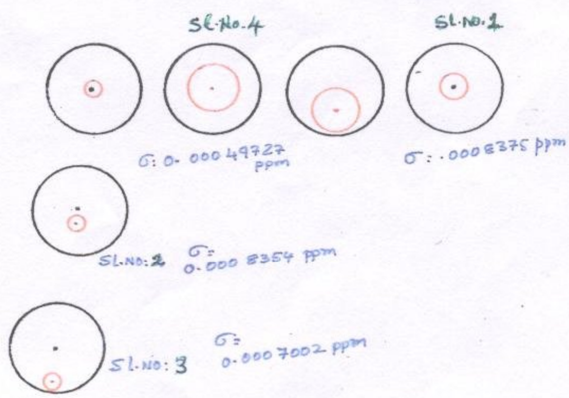
$v_{cube} = a^3$
$= 8 r^3$

$\therefore \frac{v_{cube}}{v_{sph}} = \frac{1}{\left(\frac{4 \cdot 3.14}{3} r^3\right)} \times 8 r^3$

$= \frac{1}{\frac{12.56}{3} r^3} \times 8 r^3$

$= \frac{24}{12.56} \simeq 1.9$

Hence Contribution of Sph × 1.9 gives for Cube which would Cover the voids also.



$\sigma H_0 = \left(\frac{4\pi}{3} - 4\pi \cdot D\right) H_0 \cdot \chi_v$

where D is the Demagnetization factor

$\sigma = 4\pi(1/3 - D)\chi_v$

$\frac{\sigma}{4\pi \cdot \chi_v} = 0.33 - D$

$\frac{\sigma}{12.5 \times 2.855 \times 10^{-7}} = \frac{\sigma}{35.9 \times 10^{-7}}$

for $\sigma = 0.0008375$ ppm $= 8.375 \times 10^{-10}$

$\frac{\sigma}{4\pi \cdot \chi_v} = \frac{8.375 \times 10^{-10}}{35.69 \times 10^{-7}} = 0.235 \times 10^{-3}$

$0.235 \times 10^{-3} = 0.33 - D$

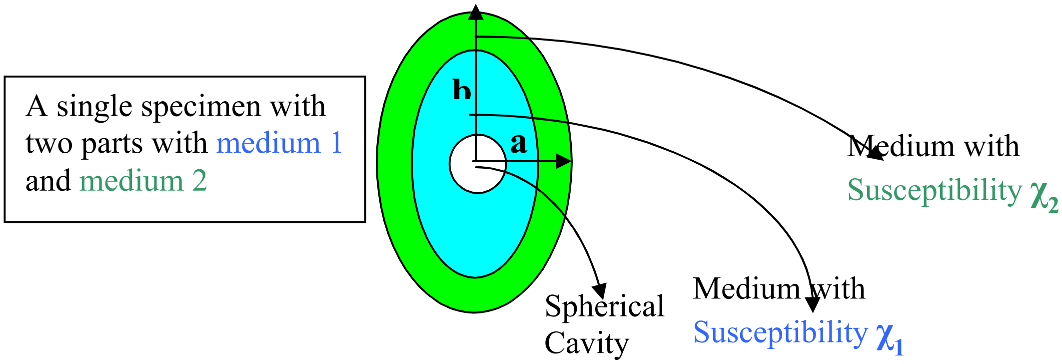
$D = 0.33 - 0.235 \times 10^{-3}$
$= 0.33 - 0.000235$
$D = 0.330235$

Advantages of the simple summation method described in the previous sheets

1. First and Foremost, it was a very simple effort to reproduce the demagnetization factor values, which were obtained and tabulated in very early works on magnetic materials. Those Calculations which could yield such Tables of demagnetization factor values were rather complicated and required setting up elliptic integrals which had to be evaluated.
2. Secondly, the principle involved is simply the convenient point dipole approximation of the magnetic dipole. And, the method requires hypothetically dividing the sample to be consisting of closely spaced spheres and the radii of these magnetized spheres are made to hold a convenient fixed ratio with their respective distances from the specified site at which point the induced fields are calculated. This fixed ratio is chosen such that for all the spheres the point dipole approximation would be valid while calculating the magnetic dipole field distribution.
3. The demagnetization factors have been tabulated only for such shapes and shape factors for which the magnetization of the sample in the external magnetic field is uniform when the magnetic susceptibility of the material is the same homogeneously through out the sample. This restricts the tabulation to only to the shapes, which are ellipsoids of rotation. Where as, if the magnetization is not homogeneous through out the sample, then, there were no such methods possible for getting the induced field values at a point or the field distribution pattern over the entire specimen. The present method provides a greatly simplified approach to obtain such distributions.
4. It seems it is also a simple matter, because of the present method, to calculate the contributions at a given site only from a part of the sample and account for this portion as an independent part from the remaining part without having to physically cause any such demarcations. This also makes it possible to calculate the field contribution from one part of the sample, which is within itself a part with homogeneously, magnetized part and the remaining part being another homogeneously magnetized part with different magnetization values. Hence a single specimen which is inherently in two distinguishable part can each be considered independently and their independent contribution can be added.

   For the point 1 mentioned above view the web page URL: http://saravamudhan.tripod.com/

An illustration of Calculation in specimen with inherently two parts



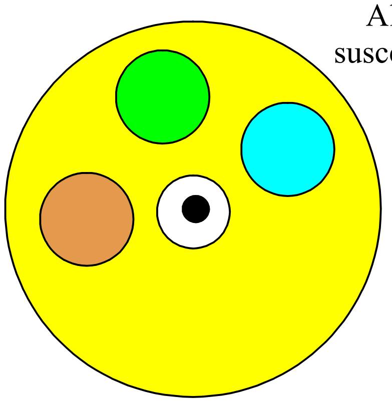
a/b	RATIO SUSC MEDIUM 1 / MEDIUM 2					
	0	**0.5**	**1.0**	**1.5**	**2.0**	**2.5**
4.0	0.071816	0.071364	0.070912	0.070461	0.070009	0.69557
3.5	0.082887	0.082436	0.081984	0.081532	0.081081	0.080629
3.0	0.105123	0.104671	0.104220	0.103768	0.103316	0.102865
2.5	0.131563	0.13111	0.130659	0.130208	0.129756	0.129304
2.0	0.169904	0.169533	0.169081	0.168629	0.168178	0.167725
1.5	0.229407	0.228955	0.228503	0.228052	0.227600	0.227148
1.0	0.329765	0.329314	0.328862	0.328410	0.327958	0.327507
0.5	0.522185	0.521734	0.521282	0.581787	0.581335	0.580883

This is a case of calculating induced field at the center of an ellipsoid [the case of **a/b=1** refers to that of a sphere with ellipticity value '**0**'**]** when the ellipsoid had concentric regions with different susceptibility values. The ratio of the susceptibility can be varied and the calculation could be done using a computer program and the entire set of data could be obtained with the program which took a run time of about 2 minutes.

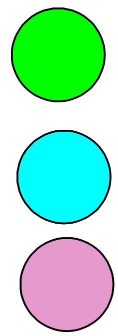
Specimens with Regional Spots of differing Susceptibility values

It should be possible for calculating the induced field contributions within a sample with Spots with varying susceptibility values even if the shape is regular ellipsoidal or which can be approximated to ellipsoid.

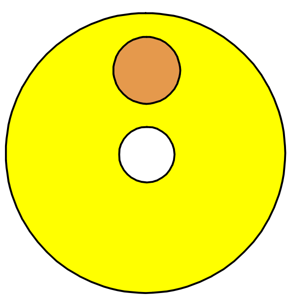
Illustartion to depict such a specimen

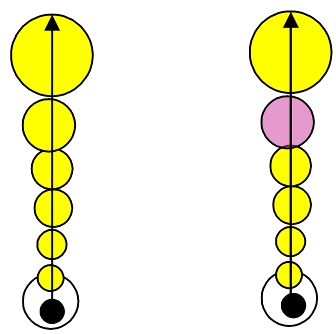


All the different colors represent different susceptibility regions within the sample.



Whenthere is such one region below:





As explained in the Sheets 7-10, along a radial vector this method would result in close packed spheres each contributing the same induced field value at the nuclear site ‘’. ‘. The●the region with susceptibilities ahs a certain number of sphere which will all would have contributed the same if the susceptibility value is the same as other spheres ‘χ_1’. But if some of these spheres have different susceptibility value then these spheres would contribute values proportionate to the ratio of the susceptibility values which means a value multiplied by χ_1 / χ_2.

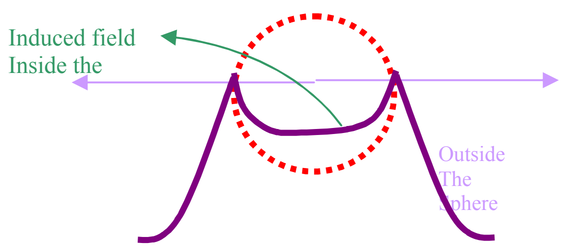
Thus along this radius vector the value can be calculated. In fact, given a length alondg this vector and the location where these sphere are placed, then using a program the number of such spheres in that length with different susceptibility values can be calculated. This could be of significance if there are floating particles with different susceptibility values.

Calculating the Induced Field at a point outside the Magnetized sphere

A consideration with a care for better insight would prop up the question whether trying to calculate the contribution at a point outside a spherical spot, as in the Sheet_13, is similar to an effort of trying to calculate the contribution to the induced field outside the spherical specimen? On the other hand , can this simple summation procedure improve the possibilities for a point dipole approximation to calculate the induced field outside the magnetized macroscopic spherical specimen ?If it does, then the considerations of other specimen shapes would fall in line for further considerations. The results depicted below indicate the advantages of this method for calculating the induced field contributions due to a specimen within and without across the sample boundaries!

Display the URL: http://geocities.com/inboxnehu_sa/icmrbs_14a.html

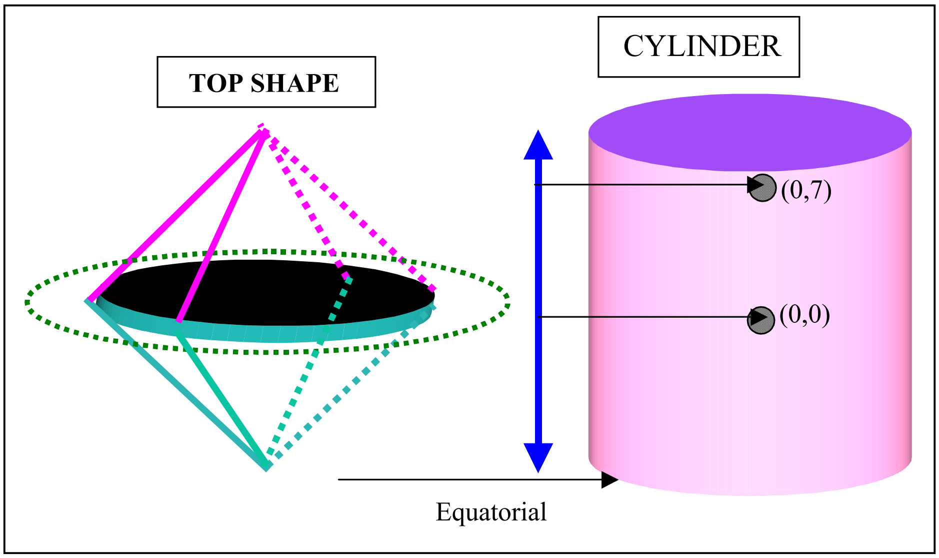
And find the descriptions as below

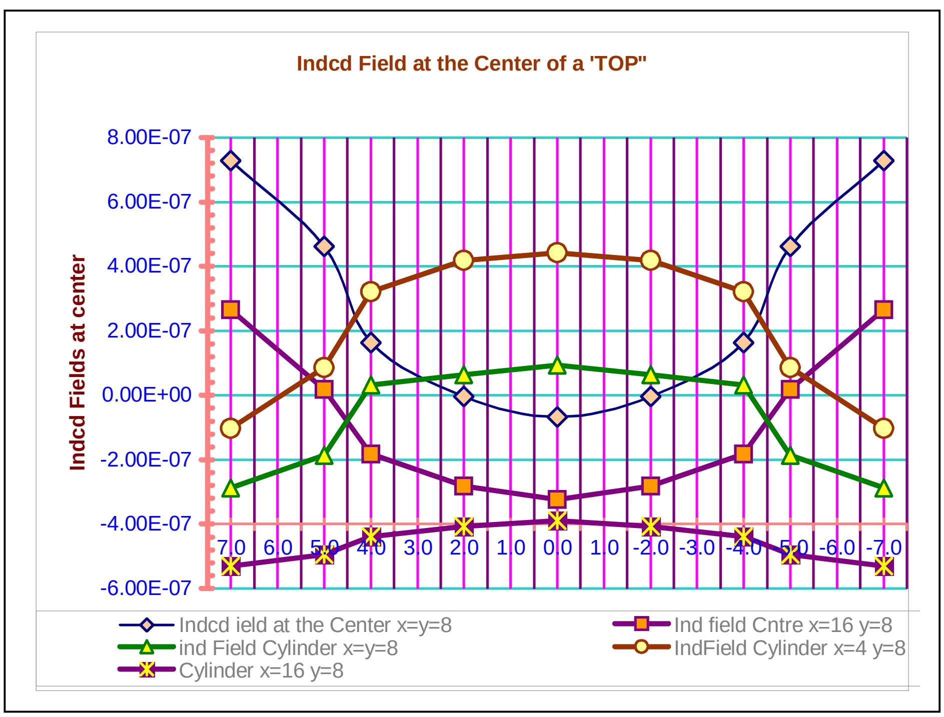


For the Graph like above the regions are as indicted herein

Possibilities for Calcualting Induced Fields for Specimen with Shapes other than Ellipsoids of Revolution

The induced Fields within the magnetized specimens for the following shapes is simple enough and the Inhomogeneous magnetization over the extene of the sample turns out to be obvious from the calculation even though the Susceptibility of the material is the same for the whole sample. The Graphical presentation of the results of these calculations are also depicetded below.





References, Summary and Conclusions

References and further materials related to the topic and the subject matter of this poster presentation can be found posted at the following Web Page URLs built by this author on the various occasions while making Progress.

http://geocities.com/inboxnehu_sa/nmrs2005_icmrbs.html

http://saravamudhan.tripod.com/id9.html

http://saravamudhan.tripod.com/id11.html

http://geocities.com/inboxnehu_sa/Poster_Sheets_Ampere.html

http://geocities.com/saravamudhan1944/eenc_ampere_lille.html

http://geocities.com/amudhan20012000/Confview_link.html

Summary and Conclusions

There have been several contexts reported in the literature for the necessities of studies by NMR techniques of the Biological Systems and the concomitant difficulties encountered because of the Bulk Susceptibility effects. All these indicate that a simpler procedure is required for calculating the induced fields due to bulk susceptibility of the medium than the hither to known mathematical procedure for the calculation of Demagnetization factors of ellipsoidal-shape magnetized specimen. As consequence of the efforts while trying to interpret the **Solid State HR PMR** data obtained by the measurements on spherically shaped single crystal specimen of organic molecules, a simpler summation procedure could evolve and was found to yield reliable and reproducible values for the calculated values of the contribution to induced field due to the Bulk susceptibility.
The various features of this simple summation procedure when carefully analyzed were found to have several features, which can be advantageous in the interpretation of NMR Spectral data, and the NMR Studies of Biological Systems had several instances where these simplifying features could be of great advantage.
In this presentation an effort has been made to list out and point out the various advantageous features and the simple method of the calculation of induced field contributions due to bulk susceptibility.
These advantageous must be appropriately used at the specific contexts in the study of the Biological Systems by NMR techniques and this may enable a more unambiguous disentangling of the various sources of induced fields at specified site and make the information more tangible for the NMR technique.
Since till now the effort has been to evolve this procedure test its reliability, reproducibility and validity for the calculations of induced fields, it is yet to find an appeal for actually applying in the Biological NMR experiments and know the simplifications this can bring in the information retrieval in the Biological Systems.