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.***

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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 approriate 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 Techniche Hochlue 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 Biopysical & 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.

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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*.

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

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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*).

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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**):

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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.

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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* **ISMAR***2013 conference included on page-6-*

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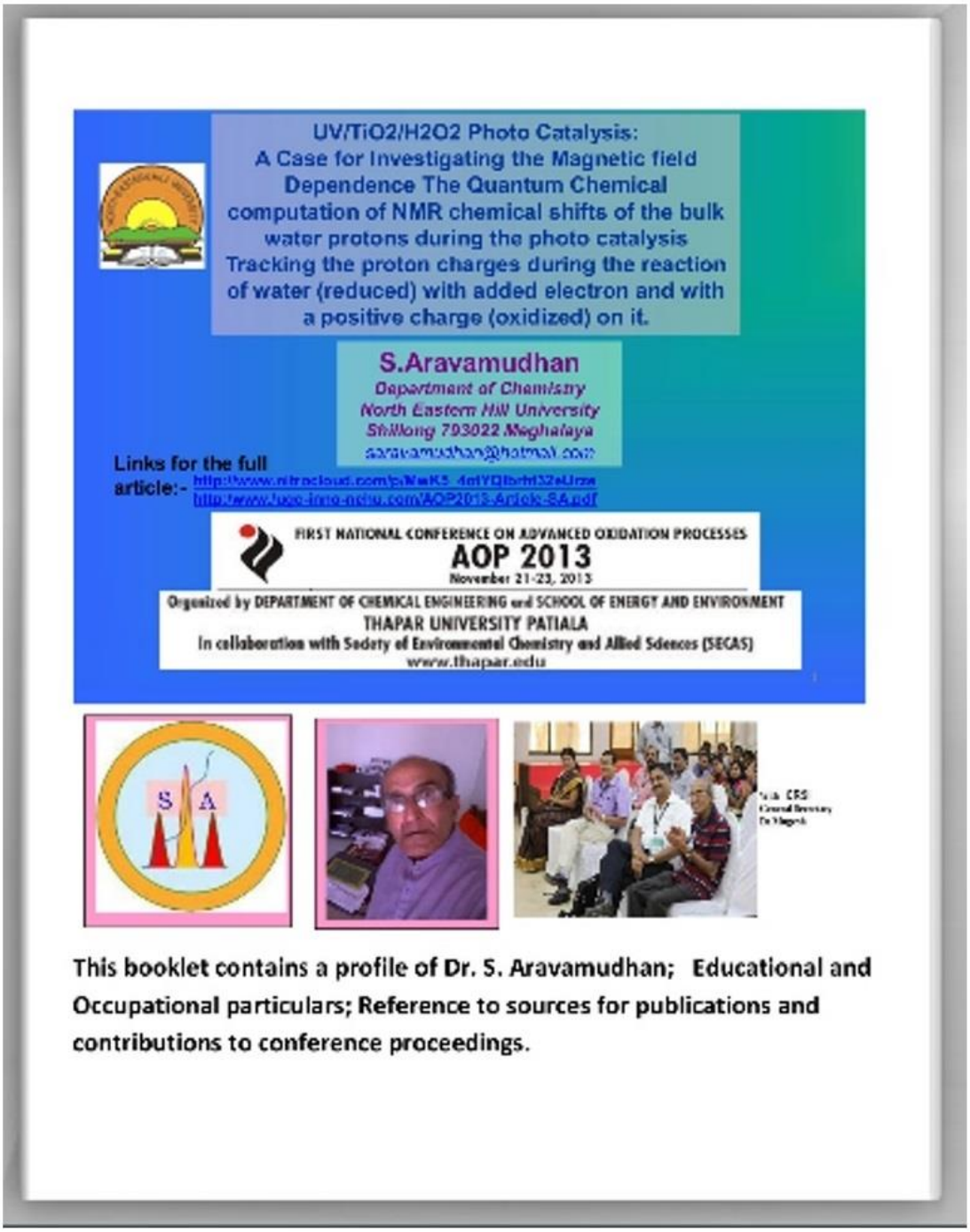

This booklet contains a profile of Dr. S. Aravamudhan; Educational and Occupational particulars; Reference to sources for publications and contributions to conference proceedings.

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