THE MICRO-MACRO PARADOX IN INDUCED FIELD CALCULATIONS AND THE ROLE OF HR SOLID STATE NMR

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A magnetized specimen can be divided into regions referred to as 'discrete' and 'continuum' regions in the context of accounting for the induced field [1] at a specified point. For such a calculation of contributions, it becomes necessary to consider the magnetic moments arising out of the magnetization of the material in a kind of average way (as elemental charge clouds circulating or as volume magnetic susceptibility value either experimentally measured or theoretically calculated) so that the contributions from these induced moments can be calculated at the center. This average magnetic property is evaluated including the corresponding material within the discrete region. Since the discrete volume element is considered separately, this amount of volume must be excluded from the total volume of the material while calculating the average. There seems an inclusion of this "small volume element around a site" (at any point within the specimen) which, paradoxically, (in particular if it is a case of non-uniform magnetization [2]) appears to have been included twice. Such kind of complications has lead to publications [3, 4] which try to explain this apparent paradox. The High Resolution NMR in Solids seems to be providing further a simplification to pursue the results on diamagnetic specimen [1].

References
[1] Magnetized Materials: Contributions inside Lorentz Ellipsoids, S.Aravamudhan, Indian Journal of Physics, Vol.79 (9), 2005, 985-989
[2] http://nehuacin.tripod.com/id3.html (4th Alpine Conference on SSNMR, 2004)
[3] Local-field Effects and Effective-medium theory, D.E.Aspnes, American Journal of Physics, 50(8), 1982, 704 to 708;
[4] Local Fields in Solids: microscopic aspects of dielectrics, S.E.Schnatterly and C.Tario, Reviews of Modern Physics, Vol. 64, 1992, 619-622.

Sheet - 4 / requires addition for elaboration

NMR SPECTROSCOPIC INVESTIGATION OF S-METHYL-N-NITROISOTIOUREA

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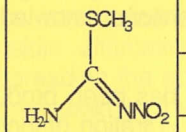
S-methyl-N-nitroisotiourea representing the interest as affective reagent for synthesis of nitroquanidine derivatives [1]. The spectral data are shown in table 1.

The temperature dependence of chemical shift of the protons of amino group in DMSO-d_6 is established (fig.1). It was also discovered the relationship between dielectric permeability and chemical shift of the protons of amino group in some solutions (fig.2).

Table 1

Compound	NMR	Chemical shifts, δ ppm.
	^1H	2,4 s. CH_3 9,1 b.s. NH_2
	^{13}C	14,4 CH_3 173,5 $C{=}NNO_2$
	^{15}N	-10,5; -112,4; -265,0 NNO_2 NNO_2 NH_2

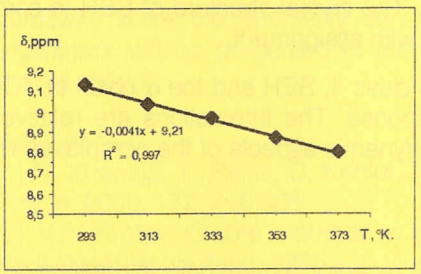


Fig.1.

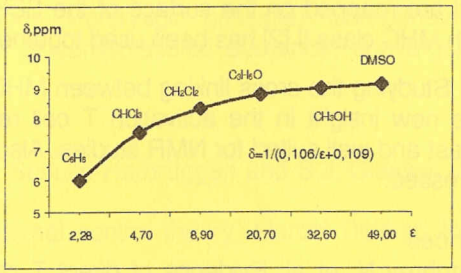


Fig.2.

References
[1] Fishbein L., Gallaghan J.A., J. Am. Chem. Soc. 1954. Vol. 76. N. 7. P. 1877–1879