

Concerning the Specimen Sample-shape for the Single-Crystal HR PMR Studies

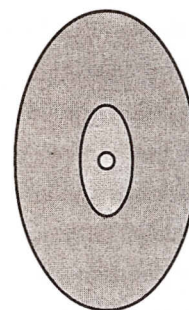
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A spherical shape for the sample has been used for the determination of Shielding Tensors of Protons in Organic Molecules in single crystal specimens by the Multiple-pulse selective-averaging techniques for NMR line-narrowing in Solid State. Ever since the break through in interpreting the experimentally measured Shielding Tensor parameters, which came about because of the possibility for taking into account the intermolecular contributions to Shielding Tensor at the site of the proton, the concerns about the necessities for the spherical shape for the sample (which is the main experimental task while trying to extend such studies as a matter of routine) became due and this was the subject matter presented (1) earlier.

It could become evident that the sample shape dependence of the experimentally determined Shielding Tensor Values can be absent if for any given regular ellipsoidal shape (frequently considered in shape-dependent bulk-susceptibility effects) if, around the proton site, a corresponding cavity could be hypothetically carved out with this cavity having the same shape factors but scaled down in size to a semimicro dimensions as in Fig. 1.

Then the question which remained to be answered was what would be the trends of the Summed up intermolecular contributions if the semimicro-volume is of an ellipsoidal shape with the corresponding shape factors as the outer specimen shape? This question could be ascertained to some extent by calculating the trends of possible limiting values as compared to the zero value for the spherical sample shape and these results (2) would be summarised. An excursion seems possible, into the further implications as to the necessity for the specified regular shapes (for reasons of Uniform magnetization of the specimen) and, into the question whether any simplification can come about for these HR PMR measurements for the other regular shapes and even arbitrary shapes in spite of the fact that the specimen would have inhomogeneous induced fields over the extent of the sample and can vary from one proton site to the other :



○ Proton Site

Fig. 1

References

1. The NMRS 2003 presentation file downloadable from http://geocities.com/amudhan_nehu/3rd_Alpine_SSNMR_Aram.html.
2. http://geocities.com/amudhan_nehu/Abstract_3rdalpine_SSNMR.html