BULK SUSCEPTIBILITY EFFECTS AND NMR CHEMICAL SHIFTS: THE PERSPECTIVE FOR MOLECULES TO MATERIALS

S. Aravamudhan

Department of Chemistry, North Eastern Hill University, Shillong, 793022 Meghalaya India

It is a well established practice to properly account for Bulk Susceptibility effects in the measurements of NMR Chemical shifts (proton chemical shifts in particular) accurately. While accounting for this bulk medium effect, it becomes necessary to consider an Inner Volume Element (I.V.E) described closer to the molecular site surrounding it which is excluded from contributions accounted for by the Bulk Medium, but the contributions within must be accounted for separately and added to the remaining contributions so that no part of the material medium gets an undue exemption from contributing to the chemical shifts. Once the above two are taken into account then the molecular contribution is determined from the experimentally measured values. The contribution from the neighbor molecules in the I.V.E. can be termed intermolecular in nature and to some extent is dependent upon the specific orientation dispositions of the neighbors, and the neighbor-molecule electronic structure. This is simply a discrete summation from individual neighbors in the case of the static orientation in Solid state single crystals. However what happens in such an I.V.E. in liquids is yet to be ascertained since even within this I.V.E., the molecules are under constant motion.

Recent results on these aspects of effect of the bulk medium in the case of diamagnetic specimen seem to provide a much clear perspective on the significance of the chemical shift determinations getting the purview from molecular to material properties of the specimen. A summary of results which highlights this significance would be given along with the specific queries to which those results stand out as clarifications.