EXPERIMENTAL DETERMINATION OF NMR TENSORS UTILIZING LCNMR SPECTROSCOPY AND COMPARISON OF RESULTS WITH THE COMPUTED ONES

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NMR spectrocopy of molecules dissolved in liquid crystals (LCNMR) is a powerful experimental means to derive elements of the nuclear shielding, indirect spin-spin coupling and quadrupole coupling tensors. This is due to the fact that the anisotropic interactions between liquid crystal and solute molecules lead to partial orientation of solute molecules which in turn causes anisotropic contributions to parameters resolvable from experimental NMR spectra. In isotropic enviroments, only averages of the respective tensors may be determined. In order to get accurate tensorial properties it is necessary, in most cases, to derive the molecular structure and orientational order parameters so completely as possible through the direct dipole-dipole couplings. This in turn necessitates the correction of the experimental dipolar couplings for vibrational and reorientational motions.
A general introduction to LCNMR will be given. Experimental results will be compared with the computed ones for some selected cases from the past (1-3) and the present (4-7).

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