Using magnetic-field induced dipolar couplings at 23.5T (1GHz for protons) to study mesogenic molecules in the isotropic phase

J.W. Emsley

School of Chemistry, University of Southampton

Mesogenic molecules in the isotropic phase experience a potential of mean torque which is too weak compared to k_BT to lead to long range orientational order. Applying a magnetic field, B, can produce a small, net orientational order along the direction of the field which may be detected optically (the Cotton-Mouton Effect), but also by NMR. Thus, magnetic-field-induced dipolar couplings become non-zero between all nuclei with non-zero nuclear magnetic moments, μ_N, and quadrupolar splittings appear for nuclei, such as deuterium, when the spin is > ½. The magnitude of these field-induced couplings depends on $\Delta\chi_{mol}$, the anisotropy in the molecular magnetic susceptibility, on B^2, and on $(T - T^*)^{-1}$. The divergence temperature, T*, lies just below T_{LC}, the temperature for the transition from isotropic to liquid crystalline phase. NMR was used to investigate the pre-transitional ordering as early as 1982 when "high field" NMR spectrometers, with B = 9.3T, first became available, using deuterium NMR. The quadrupolar splittings observed were appreciable, but were accompanied by a large field-induced line broadening, which also diverged towards T*. Interest waned, partially because of this large line broadening, which made spectral analysis difficult, but also because of the necessity of specifically labelling the mesogens with deuterium. The ability to measure field-induced dipolar couplings has now become possible with the advent of spectrometers operating at "very high fields", and here we show results of proton and carbon-13 spectra taken on a 1 GHz spectrometer. At this field large sets of field-induced dipolar couplings can be obtained without the need for isotope labelling.