Endofullerenes in Liquid Crystals

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By dissolving endohedral fullerenes $N@C_{60}$ and $N@C_{70}$ in liquid crystals, the alignment of these nearly spherical objects can be studied with EPR techniques. As example results obtained using the nematic phase of 4-Methoxybenzylidene-4’-n-butylaniline (MBBA) and Merck ZLI-1965 are presented. For both probe molecules well resolved EPR spectra give proof for molecular orientation in the nematic mesophases. Spectral features are dominated by a non-vanishing zero field interaction, indicating a deviation from spherical spin density distribution at the encased nitrogen atom. In $N@C_{70}$, the order parameter O_{33}, which is correlated with the long axis of the cage, and the Zero-Field-Splitting parameter D could be quantitatively determined. For both solute molecules we observed a change of the order parameter when using ZLI-1965 in stead of MBBA, indicating the dominance of long range solvent/solute interactions. In case of $N@C_{60}$, only the product of O_{33} and D can be measured, which shows the same temperature dependence as found for $N@C_{70}$. An assignment of the director with respect to the molecular frame of $N@C_{60}$ is not possible, the observed line splittings, however, being indicative of pseudo orientation of the rapidly rotating cage.