Orientation and dynamics of benzyl alcohol and benzyl alkyl ethers dissolved in nematic lyotropic liquid crystals.2H NMR and molecular dynamics simulations

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The distribution, orientation, and dynamics of benzyl alcohol and benzyl ethers dissolved in nematic lyotropic liquid crystals were analyzed using nuclear magnetic resonance (NMR) and molecular simulations. The molecules were dissolved in a nematic discotic lyotropic liquid crystal solution made of tetradecyltrimethyl-ammonium chloride (TTAC)/decanol. Rotational correlation functions of all the C-D bonds and the OH bond from H2 were evaluated, allowing an estimate of the correlation times and T1. The results show that the existence of a dynamic process reorienting the ring symmetry axis averages the quadrupole splittings from ortho and meta positions in the ether series.