Dynamics of Liquid Crystals by Means of ²H-NMR: a Comparison between 4,4'-bis(hexyloxy)azoxybenzene and the Derivative Pd(II) Complex AZPAC*

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In the present work we report a molecular dynamics investigation of the two mesogens 4,4'-bis(hexyloxy)azoxybenzene (HL) and its Pd(II) acetylacetonate derivative Azpac in their nematic phases. Deuterium Zeeman and quadrupolar spin-lattice relaxation times have been measured at 46.04 MHz on two isotopomers of Azpac (Azpac-d₄ and Azpac-d₂₆, deuteriated on the aromatic core and on the alkoxy chains, respectively) and on HL-d₄, an isotopomer of HL partially deuteriated on the aromatic core, by means of the Wimperis pulse sequence. The spectral densities obtained from the measured relaxation times are discussed in terms of internal and overall molecular motions. A small step rotational diffusion model for the overall molecular motions, superimposed on a free rotational model for internal motions, allowed diffusion coefficients for molecular spinning and tumbling and for phenyl ring rotations to be derived for HL; the same models were used in describing the dynamics of Azpac.

Key words: Liquid Crystals; Deuterium Relaxation; Molecular Dynamics; Metallomesogens; NMR.

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