

European Network on NMR Relaxometry

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The solvent dynamics at pore surfaces in molecular gels studied by FFC relaxometry

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The field-cycling NMR relaxometry has been used to identify and characterize the molecular dynamics in low molecular mass gels and in bulk solvents. The gels are made by 4,6,4',6'-O-terephthalylidene-bis(methyl α -D-glucopyranoside gelator with ethylene glycol (EG) and 1,3-propanediol (PG) and prepared with different gelator concentrations. The spin-lattice relaxation dispersion data of proton solvents in bulk were analyzed assuming the intramolecular and intermolecular dipole–dipole interactions. The two-phase fast-exchange model was used for the analysis of the relaxation data for PG and EG solvents confined in the gel. We assumed that in a low-frequency range, the reorientation mediated by translational displacements (RMTD) is the dominating NMR relaxation mechanism of the solvent molecules interacting with internal surfaces of the pores. The RMTD contribution to the relaxation is described by power-law frequency dependence. In the 1/EG gels, the exponent is equal to 0.5 for all gelator concentrations suggesting the equipartition of the diffusion modes with different wavelengths. In the 1/PG gel, the exponent varies in the function of gelator concentration. The different behavior of the relaxation dispersion shape is due to the relative sizes of the ordered (at the surface) and bulk-like phase. In the 1/EG gel, the surface layer of the ordered molecules is always much smaller than the dimensions of the gel cavities whereas it differs in the 1/PG gel as a consequence of the disruption of the PG aggregates due to the solvent–gelator interaction. The RMTD dynamic process allows us to explain a very long correlation time of the order of 10^{-5} s calculated for confined EG molecules and an even longer one for PG confined molecules.

J. Tritt-Goc, A. Rachocki, M. Bielejewski, *Soft Matter*, 2014, 10, 7810