MULTIDIMENSIONAL LAPLACE NMR RELAXATION AND DIFFUSION STUDIES OF A PHOSPHONIUM BIS(MANDELATO)BORATE IONIC LIQUID

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Ionic liquids (ILs) are molten salts that solely consist of ions and exhibit high ionic conductivity. The unique properties, *i.e.*, negligible vapor pressures, low flammability and high liquid ranges, thermal stabilities, as compared to other molecular solvents, make ionic liquids a topic of interest for researchers in academia as well as in industry. Halogen-free, boron based ionic liquids composed of chelated orthoborate anions and phosphonium cations exhibit good lubrication properties including wear and friction reducing potential, low melting points and a high thermal and hydrolytic stability [1]. Interestingly, one of these ILs, trihexyltetradecylphosphonium bis(mandelato)borate, $[P_{6,6,6,14}]$[BMB], has shown two significantly distinct diffusion coefficients at temperatures below 340 K, which was explained by the presence of two percolated liquid phases in the IL and could, in turn, be correlated with outstanding friction and wear reducing properties of this IL [2].

NMR relaxation and diffusion experiments provide versatile information about the dynamics and structure of substances such as ionic liquids, proteins, polymers, liquid crystals and porous media. They also improve the chemical resolution by separating different components in complex systems without spectral resolution. Multidimensional experiments greatly enhance the chemical resolution and information content in NMR relaxation and diffusion studies [3].

The present Laplace NMR T_2 relaxation and diffusion studies aim to characterize, by means of variable temperature, the structural phases of $[P_{6,6,6,14}]$[BMB] IL. The presence of two distinct T_2 components suggests that there exist at least two phases at lower temperatures and a single homogeneous liquid phase at higher temperatures above 340 K. At lower temperatures, T_2-T_2 and D-D exchange experiments reveal the exchange between two sites informing about the exchange rate between two components, while D-T_2 correlation experiments correlate the transitions of coupled spins by transferring coherences from one transition to another. The D-T_2 correlation experiments reveal that the slow diffusing component has higher relaxation rate while fast diffusing component has smaller relaxation rate.

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