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Polymorphism and dynamics of neohexanols studied by NMR spectroscopy and relaxometry

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Neohexanol (2,2-dimethyl-1-butanol, $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$) and some of its isomers, differing for the positions of the OH and CH_3 substituents, constitute a very interesting class of compounds showing a rich polymorphism with several solid-solid phase transitions. Indeed, due to their globular shape and to the possibility to associate through hydrogen bonds, at low temperatures they give rise to both plastic crystalline phases and glasses. In particular, some of these compounds show orientationally disordered crystals (ODIC) due to the ease of rotational motions of the molecules in the solid state [1].

Fast field cycling (FFC) NMR relaxometry is a very important technique for obtaining information on dynamic properties, allowing internal, overall and collective molecular motions to be investigated by means of measurement and analysis of ^1H longitudinal relaxation times over a wide Larmor frequency range (10 kHz – 40 MHz). In particular, ^1H FFC NMR relaxometry has been successfully applied in the study of motions related to the glass transition process in viscous liquids and polymers [2]. On the other hand, solid-state NMR spectroscopy is a very powerful technique for the study of dynamics, providing, through a combination of different experiments and observable nuclei, complementary information with respect to FFC NMR.

In this work ^1H FFC NMR relaxometry and solid-state ^1H and ^{13}C NMR experiments have been applied to neohexanol and three of its isomers (3,3-dimethyl-2-butanol, 2,3-dimethyl-2-butanol and 3,3-dimethyl-1-butanol) in the temperature range from -60 to 30 °C. In particular, ^1H spin lattice relaxation times ($T_{1\rho}$) have been measured at Larmor frequencies from 10 kHz to 35 MHz with FFC techniques and at 400 MHz with Saturation-Recovery experiments. Moreover, static ^2H and ^{13}C NMR spectra have been recorded under ^1H high-power decoupling. The spectroscopic and relaxation data acquired for the different isomers have been compared and analyzed to obtain information on the dynamic processes occurring in the different solid phases as well as to establish relationships between chemical structure and dynamic properties.

References

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