

Dynamics of molecular crystals by means of ^1H NMR relaxometry: dynamical heterogeneity versus homogenous motion.

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(^1H) NMR relaxometry was used to reveal information on the dynamical properties of the molecular crystal $(\text{PyH})_5 \text{Bi}_2 \text{Br}_{11}$ ($\text{PyH} = \text{C}_5\text{H}_6\text{N}$, pyridinium cation), chosen as an example of a solid that exhibits a complex structure and rotational-like dynamics. Experimental studies were performed over a very broad frequency range, from 4 kHz to 40 MHz (referring to the (^1H) resonance frequency) versus temperature. The extensive set of data was thoroughly analyzed in terms of two motional models differing with respect to the assumed mechanism (heterogeneous versus homogenous) of the motion of the PyH cations. A Cole-Davidson distribution of the correlation times describing the assumed motional heterogeneity was tested against a concept of two correlation times characterizing the rotation-like dynamics of the PyH cation around the perpendicular axes differing by about one order of magnitude. The parameters describing the dynamics of the cation, obtained by means of both models, were compared and discussed.

Słowa kluczowe

molecular crystals, molecular dynamics, NMR spectroscopy, relaxation, solids

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